University of Reading

Department of Mathematics and Statistics

Numerical solution of an ODE system arising in photosynthesis

Author:
Rabindra GURUNG

Supervisors:
Prof. Mike BAINES
Dr. Peter SWEBY

A thesis submitted in partial fulfilment of the requirements for the degree of

MSc in Applicable and Numerical Mathematics

August 17, 2014

Abstract

A simple model of light use in the Photosystem II model of Photosynthesis by leaf under light changing condition has been studied using a system of three nonlinear ordinary differential equations (ODEs). As part of our analysis we show that there is a unique stable solution. We identify a stiffness problem and have solved the system of ODEs using a stiff solver $ode23s$, and compared the results with a previous solution using explicit Euler scheme. We also describe an asymptotic analysis of the system of 3 ODEs and consider sensitivity to particular unknown parameters used in the ODEs. In the model [1] one of the equations proceeds very rapidly which allows the system of 3 ODEs to be reduced to a system of 2 ODEs. We compared both systems of ODEs by looking at the steady-states, stability and stiffness of the systems. We have numerically approximated the governing differential equations and compared results with each order.

Acknowledgements

“Great people make you feel that, you too, can become great.” This quote originates with Mark Twain and carries much truth.

My first acknowledgment is to my academic supervisors, Prof. Mike J Baines and Dr. Peter K Sweby for all the help, time and advise that they have given me throughout this project and over the MSc year. I am extremely grateful for the careful attention, patience and support I received from my advisors. I would also like to acknowledge the other staffs and students in the Mathematics and Statistics department.

Finally, I would like to thank my family and friends, for their love and support given me to take full advantage of this wonderful opportunity.

Declaration

I,RABINDRA GURUNG, declare that this dissertation titled, ‘Numerical solution of a stiff ODE system arising in photosynthesis’ and the work presented in it are my own. I confirm that the use of all materials from other sources has been properly and fully acknowledged.

Signed: ____________________________________

Date: ____________________________________

List of Figures

List of Tables

Contents

Chapter 1

Introduction

This dissertation is concerned with the numerical solution of a system of nonlinear ordinary differential equations (ODEs) which arise in photosynthetic dynamics due to light variation, which has been investigated experimentally in dark and light [1] [2].
In the next section we summarize the available information on photosynthetic response to light variation and derive a mathematical model for a dynamic approach for leaf response under high and low light conditions.

1.1 Background of Study

By capturing the energy of sunlight and converting it into chemical potential energy, photosynthesis powers most life on earth [3]. Light is obviously a key ingredient in photosynthetic energy capture. Under natural fluctuations in light environments, on most days plants encounter light intensities that exceed their photosynthetic capacity [5]. Excessive light energy can damage the photosynthetic membranes and machinery of the plants. Plants have therefore developed mechanisms that can quickly and effectively repair photo damage. To better understand the mechanism of the excessive capacity of leaves, the model [2] compares a dynamic approach with a steady-state approach.

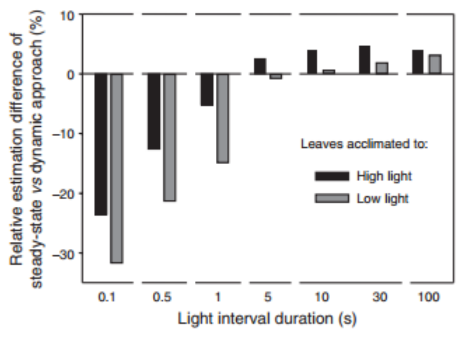

Figure 1.1: Comparison of steady-state and dynamic approach taken from [2].

Figure 1.1 presents a comparison between steady-state and a dynamic approaches under light intensity between high light ($1500 \mu mol m^{-2} s^{-1}$) and low light ($100 \mu mol m^{-2} s^{-1}$) [2]. Study of figure 1.1 shows that in those conditions where the light intensity changes faster than $1s$ the steady-state approach significantly underestimates the modified electron transport [2]. The effect reverses every few seconds, where the steady-state approach overestimates compared with dynamic approaches. Considering this behaviour, the paper [2] concluded that a steady state approach might lead to overestimation in leaves at the top and underestimation at the lower part of leaves.

1.1.1 Photosystem II

One of the first states of photosynthesis involves a process called photosystem II [3]. The oxygen we breathe is a product of photosystem II reactions. Photosystem II is made up of many different proteins and pigment molecules . The heart of photosystem II is the reaction centre [3], where the energy of light is converted into the motion of energized electrons. It captures photons with the help of two types of chlorophyll, chlorophyll a ($Chla$) or chlorophyll b ($Chlb$), molecules where $Chlb$ operates only in light absorption and excitons are always assumed to be located in $Chla$ [2]. The various process that compete for light energy absorbed by a leaf for Photosystem II are [2]

- photochemistry,
- fluorescence,
- non-photochemical quenching,
- heat dissipative process.

The main energy-consuming processes in photosystem II are often classified into photochemical and non-photochemical processes. Photochemistry is the energy that gives fuel for photosynthesis [1]. Fluorescence and heat dissipation are used for non-photochemical processes which utilities the absorbed light energy. Non-photochemical quenching occurs when there is an increase in the rate at which excitation energy within photosystem II is lost as heat. The background mentions that high light is a major stress for plants. One of the strategies for survival in high light is to eliminate the excess absorbed energy as heat thermal dissipation which can be measured as non-photochemical quenching(NPQ) for chlorophyll fluorescence [4]. NPQ processes can be thought of as protective mechanisms of the plant to cope with excess heat excitation. Chlorophyll fluorescence techniques are widely used to study the dynamics of the energy-consuming processes [2] in photosystem II .

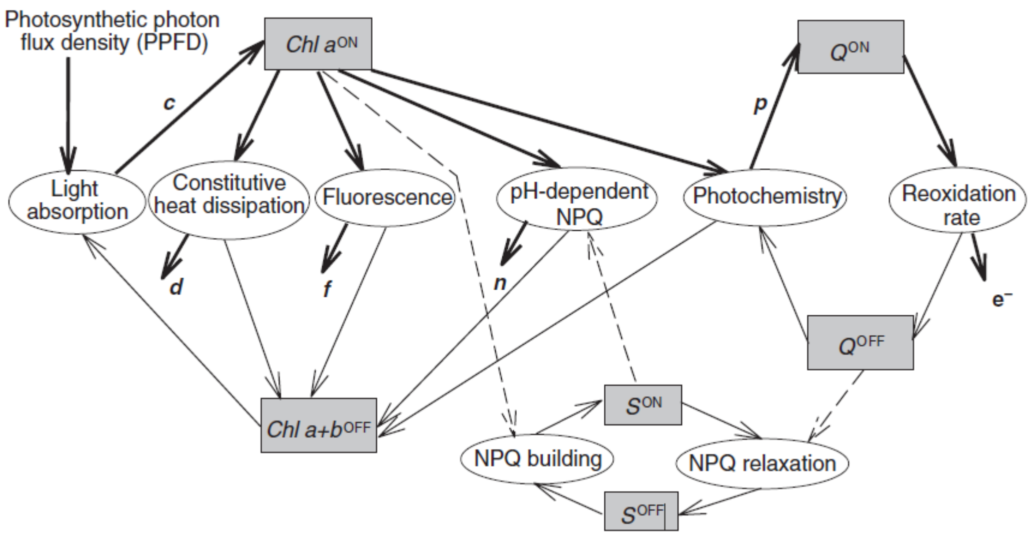

Figure 1.2: Process of photosystem II taken from [2].

Rectangular boxes represent amounts of a substance in a determined state, and ellipsoids represent processes where absorbed light can be utilised [2]. Thick arrows represent the flow of energy, and broken arrows indicate an effect. $Chla^{ON,OFF}$ represents molecules carrying an exciton(ON) or in the ground state (OFF) [2]. $Chla + b^{OFF}$ is the sum of chlorophyll a and b molecules in the system in the ground state [2]. $Q^{ON/OFF}$ are the number of photochemical quenching in reduced or oxidised state [2]. $S^{ON/OFF}$ are the number of active or inactive non-photochemical quenching sites. d, f, n and p are the rates of constitutive heat dissipation, fluorescence, non-photochemical quenching processes and reduction of the quinone-equivalents, respectively [2].

In the study [2] the model is concerned with the steady state for light reaction which may encounter problem under natural fluctuating light. So, by developing a dynamic model can express the behaviour of the system over short time periods can be expressed.

1.2 Objectives of the study

We study a system of three ordinary differential equations (ODEs) that arise in the model of photosynthesis reaction. The system of 3 ODEs is nonlinear and has no analytical solution. We investigate steady-state solutions and their stability but also the process under which the solution reaches these steady-states. The main purpose of this study is to develop efficient numerical methods to get the results.

The objectives of the study are

- to study the steady-states, stability and stiffness of the system,
- to get accurate and stable solutions by solving the system numerically using ode solver $ode23s$ of MATLAB,
- to study the initial asymptotic behaviour of the system,

- to discuss the sensitivity of unknown parameters of the system.

In the model [1], based on [2], the systems of 3 ODEs is reduced to a system of 2 ODEs and we compare the results between the 3 and 2 ODEs systems in terms of steady-states, stability and stiffness. We also compare the results of the system of three ODEs solved by a stiff solver $ode23s$ with the previous results of the model [1] solved using the Explicit Euler scheme.

1.3 Structure of Dissertation

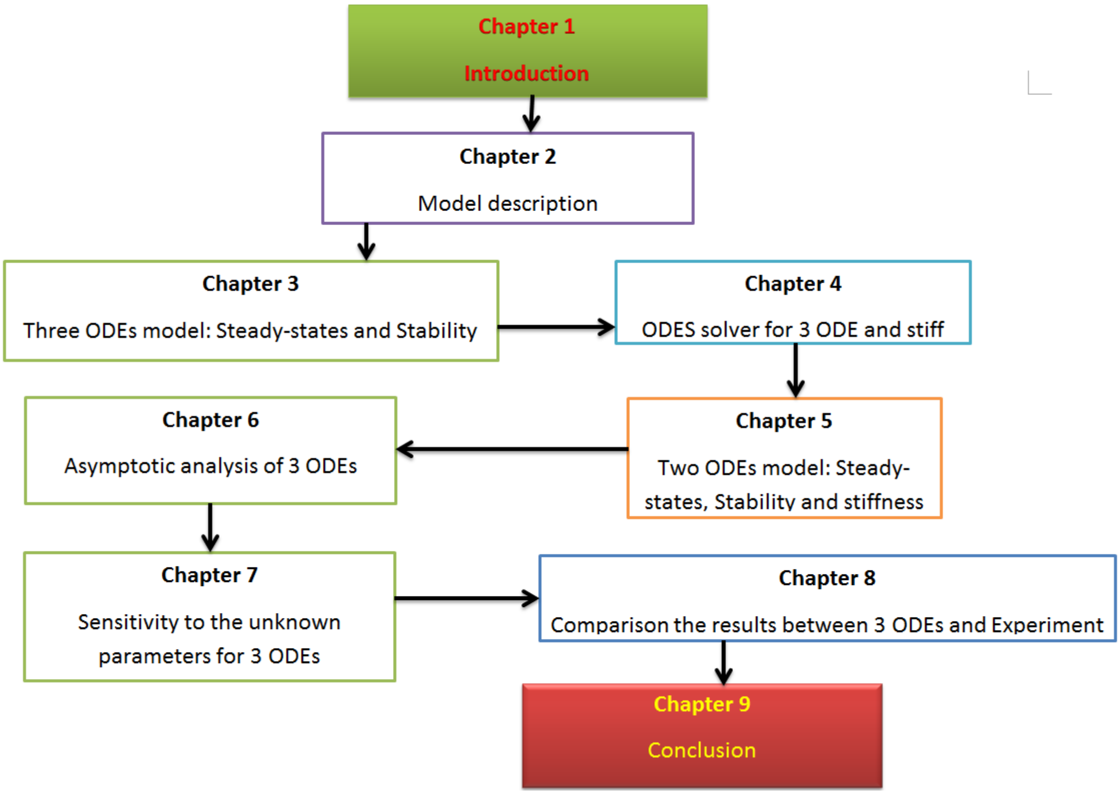

Figure 1.3: Dissertation Structure roadmap.

Before beginning to present our methods, in Chapter 1 we discuss the main paper *"Dynamic flow of energy through Photosystem II under light changing conditions"* [2] which provides the background of our study to show how plants react under high or low light in photosystem II and compare steady-states and dynamic approaches to the system. It describes the process of Photosystems II and then reviews the objectives of this dissertation.

Chapter 2 includes the model description from the associated note "A simple model of light use in Photosystem II" [1]. We review this model [1] that has already been carried through on the nonlinear system of three ODEs which includes a numerical experiment under light changing conditions using the Explicit Euler method. In the section (2.1) of this chapter, we describe a non dimensionlization of the 3 ODEs to simplify the system and meaning of the parameters used in the equations.

Chapter 3 determines the steady-states of the system of 3 ODEs using a Newton-Raphson method and Descartes rule of signs, to show there is only one positive stable steady-state solutions which lies between 0 and 1. Then we will analysis the stability of the steady-states of the system.

In Chapter 4 we discuss the stiffness of the 3 ODEs by finding the condition number of the Jacobian at the start of the experiment and then use the ode solver $ode23s$ to solve the system of 3 ODEs. We then move on to the system of 2 ODEs.

Chapter 5 considers the reduced system of 2 ODEs, which does not contains the initial stiff behaviour of c. We again find the steady-states, stability and stiffness of the system of 2 ODEs and compare them with the system of 3 ODEs.

In chapter 6 we turn our attention to an asymptotic analysis of the 3 ODEs close to initial states and compare the results with the numerical behaviour of system of the 3 ODEs in a very small time.

In chapter 7 we look at the sensitivity of the system to some unknown parameters and measure the differences between the results using the perturbed and actual values of these unknown parameters.

In chapter 8 we compare the results from 3 ODEs obtained from the ode solver $ode23s$ against the results of model [1] obtained by the Euler scheme to check the steady solutions got from both methods.

The summary and main results of all the work reported in this thesis are contained in chapter 9. Finally we draw the conclusion from the two numerical methods and all the results we have obtained and propose some questions to be answered in future work.

Chapter 2

Model description

The paper [2] [1] entitled *"A simple model of light use in Photosystem II"*, by A. Porcar-Castell studies what happens to light energy after it has been absorbed by a leaf but before it has been used in photosynthetic reactions. The model comprises a system of three nonlinear ordinary differential equations. In the model [1] there are 3 main populations of molecule -type entities which are

1. $Chla$
2. S
3. Q.

The total amount of each of these entities is conserved. Q and S are biochemical states of the systems [1]. All these three entities are important during the process of photosystem II after absorbing the light energy. The flux of energy through the systems is controlled by the system of differential equation.

2.1 System of 3 differential equations

From the figure 1.2, during the process of photosystem II for the rate of light capture by the chlorophyll a molecule since chlorophyll b molecule do not locate the exicitons [2]. The energy enters the system of differential equations and is split between the competing downstream processes as $Chla^{ON} + Chla^{OFF}$ where $Chla^{ON}$ satisfies

$$\frac{dChla^{ON}}{dt} = \alpha IChla^{OFF} + Chla^{ON}(-k_f - k_d - k_n E - k_p Q). \tag{2.1}$$

Non photochemical processes are modelled as

$$\frac{dS^{ON}}{dt} = \lambda_b Chla^{ON} S^{OFF} - \lambda_r Q S^{ON} \tag{2.2}$$

where the total S pool size is $S^{OFF} + S^{ON} = constant.$

Photochemical processes are modelled as

$$\frac{dQ^{ON}}{dt} = k_p Q Chla^{ON} - \gamma Q^{ON} \tag{2.3}$$

where the total Q pool size is $Q^{OFF} + Q^{ON} = constant$.

The process in equation 2.1 occurs rapidly and therefore we set the derivative to zero and rearranged to yield

$$Chla^{ON} = \frac{\alpha I Chla^{OFF}}{k_f + k_d + k_n E + k_p Q}.$$

E is biochemical states of the systems [1].
The variable E refers to the fraction of S in the ^{ON} state

$$E = \frac{S^{ON}}{S^{OFF} + S^{ON}}. \tag{2.4}$$

The variable Q refers to the fraction of Q in the ^{OFF} state

$$Q = \frac{Q^{OFF}}{Q^{OFF} + Q^{ON}}. \tag{2.5}$$

The meaning and values of parameters used in the system of differential equations are presented in the following tables.

name	what?	meaning	unit
I	input	incident light	$\mu E m^{-2} s^{-1}$
α	parameter	light capture efficiency	$m^2 chl^{-1}$
k_f	parameter	rate constant fluorescence	s^{-1}
k_n	parameter	rate constant non photochemical quenching	s^{-1}
k_p	parameter	rate constant photochemical quenching	s^{-1}
k_d	parameter	rate constant other heat	s^{-1}
γ	parameter	controls photochemical building	n/a
λ_b	parameter	controls non photochemical building	n/a
λ_r	parameter	controls non photochemical relaxation	n/a
$Chla^{ON/OFF}$	state	number of excitons in state $^{ON/OFF}$	n/a
$S^{ON/OFF}$	state	number of NPQ entities in state $^{ON/OFF}$	n/a
$Q^{ON/OFF}$	state	number of PQ entities in state $^{ON/OFF}$	n/a

Table 2.1: Parameters and their meanings taken from [1].

Rate constant or parameter	Value
$k_f(s^{-1})$	6.7×10^7
$k_n(s^{-1})$	6.03×10^8
$k_p(s^{-1})$	2.92×10^7
$k_d(s^{-1})$	4.94×10^7
γ	2.74
λ_b	0.0087
λ_r	835
I $(\mu mol m^{-2} s^{-1})$	1200
α	1.14437×10^{-3}

Table 2.2: Values of parameters associated with energy processes in PSII taken from [2].

2.2 Non dimensionlization

Non-dimensionlizing the system of nonlinear ODEs is important because it simplifies the equations and allow us to analyze the behavior of the system with the values of variables ~ 1.

The system of differential equations are

$$\frac{dChla^{ON}}{dt} = \alpha I Chla^{OFF} + Chla^{ON}(-k_f - k_d - k_n E - k_p Q). \tag{2.6}$$

$$\frac{dS^{ON}}{dt} = \lambda_b Chla^{ON} S^{OFF} - \lambda_r Q S^{ON} \tag{2.7}$$

$$\frac{dQ^{ON}}{dt} = k_p Q Chla^{ON} - \gamma Q^{ON} \tag{2.8}$$

Letting P_C be the pool size of $Chla$, non dimensionalise $Chla$ as

$$\frac{Chla^{ON}}{P_C} = c, \; \frac{Chla^{OFF}}{P_C} = 1 - c,$$

S as

$$\frac{S^{ON}}{P_S} = s, \; \frac{S^{OFF}}{P_C} = 1 - s \tag{2.9}$$

Q as

$$\frac{Q^{ON}}{P_C} = q, \; \frac{Q^{OFF}}{P_C} = 1 - q \tag{2.10}$$

where,

$$P_C = Chla^{ON} + Chla^{OFF},$$
$$P_S = S^{ON} + S^{OFF},$$
$$P_Q = Q^{ON} + Q^{OFF}.$$

c, s and q are the non-dimensionalised variables which lies between 0 and 1.

Using equation (2.4), we substitute for S^{ON} and S^{OFF} from (2.9) into variable E and to give

$$E = \frac{P_S\ s}{P_S(1-s) + P_S\ s}$$

so that

$$E = s.$$

Using equation (2.5), we substitute for Q^{ON} and Q^{OFF} from (2.10) into variable Q giving

$$Q = \frac{P_Q(1-q)}{P_Q(1-q) + P_Q\ q}$$

so that

$$Q = (1-q).$$

The system of equations (2.6), (2.7) and (2.8) then becomes,

$$P_C\frac{dc}{dt} = \alpha I P_C(1-c) + P_C\ c(-k_f - k_d - k_n s - k_p(1-q)),$$

$$P_S\frac{ds}{dt} = \lambda_b P_C\ cP_S(1-s) - \lambda_r(1-q)P_S\ s,$$

$$P_Q\frac{dq}{dt} = k_p(1-q)P_C\ c - \gamma P_Q\ q,$$

which can be rearranged as

$$\frac{dc}{dt} = \alpha I(1-c) + c(-k_f - k_d - k_n s - k_p(1-q)). \tag{2.11}$$

$$\frac{ds}{dt} = \lambda_b P_C\ c(1-s) - \lambda_r(1-q)\ s. \tag{2.12}$$

$$\frac{dq}{dt} = k_p(1-q)\frac{P_C}{P_Q}\ c - \gamma\ q. \tag{2.13}$$

We will be using the non-dimensionalized nonlinear equations to seek the results of the systems.

In the model [1], the ratio of pool values are $230 : P_C = 22 : P_Q$.
From figure (2.1), pool value $(P_C) = 3e^{11}$ then value of P_Q is given by

Pool Values	Meanings	Values
P_C	$Chla^{ON} + Chla^{OFF}$	3×10^{11}
P_Q	$Q^{ON} + Q^{OFF}$	Ratio of $230 : P_C = 22 : P_Q$ gives $\frac{22 \times 3e^{11}}{230} = 2.87 \times 10^{10}$

Table 2.3: Values and meanings of pool values.

In the next section, using the values of parameters and pool values from tables (2.2) and (2.3) into system of 3 ODEs the experiment was conducted under light changing conditions.

2.3 Experiment and Results from previous work

- Dark reactions

In [1] a simulation was conducted using the Explicit Euler scheme on the 3 ODEs by keeping the leaf in the dark at least for 2 hours. With knowing some knowledge of pool size through pigment measurement then estimation can be done for all the relevant initial conditions. Coefficient Q which refer to photochemical process will rise to 1 where as coefficient E which refer to non-photochemical process will fall to 0.

- Light reactions

After that shine a constant light on the leaf and watch out what happens to the the dynamics of energy flow under changing the light conditions as shown in figure 2.1.

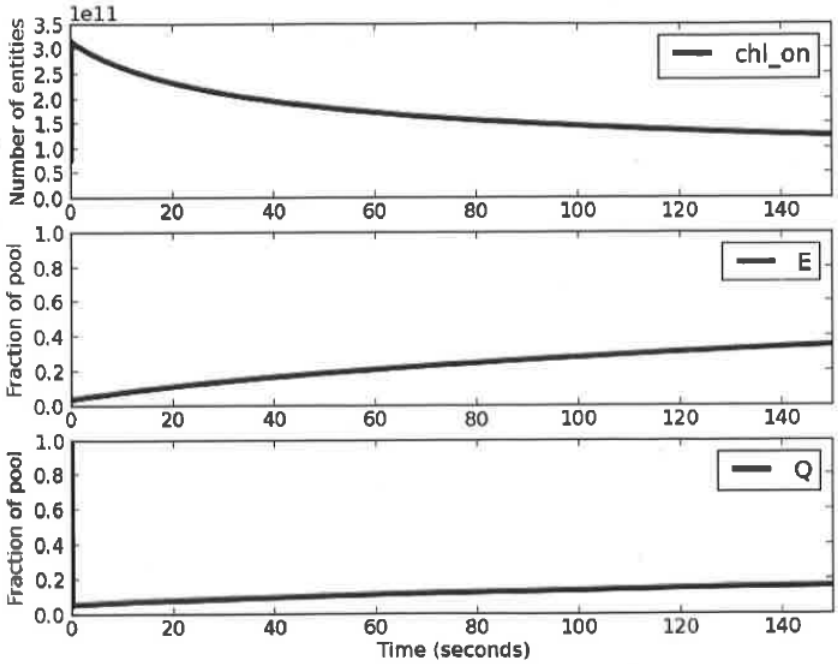

Figure 2.1: Single Model run with initial conditions and constant irradiance taken from [1].

In the figure 2.1 the model of 3 ODEs was run using the Explicit Euler scheme with the help of initial conditions and constant light shinning on the leaf. It shows how the 3 molecules $Chla^{ON}$, Q and E behave under the changing light conditions. The initial condition of Q starts from 1 and E starts approximately from 0 because it uses the final value for Q and E in the dark reaction and it becomes the initial value in the light reaction after the light comes on. The model is initially derived to account for dark reaction to light reaction and all the parameters used in the equations of ODEs were tested under chlorophyll fluorescence data [2]. The aim of this study was to develop a dynamic model of the energy flow in photosystem II under changing light conditions occurring at a time scale of seconds to minutes [2].

Chapter 3

Three ODEs model: Steady-states

In this chapter, we begin by looking for steady states of the 3 ODEs (2.11), (2.12) and (2.13), i.e.

$$\frac{dc}{dt} = \alpha I(1-c) + c(-k_f - k_d - k_n s - k_p(1-q)),$$

$$\frac{ds}{dt} = \lambda_b P_C \ c(1-s) - \lambda_r(1-q) \ s,$$

$$\frac{dq}{dt} = k_p(1-q)\frac{P_C}{P_Q} \ c - \gamma \ q$$

where the meaning of parameters and pool values used in the equations are taken from the tables (2.1) and (2.3).

The steady-states of the systems are given by

$$\frac{dc}{dt} = 0,$$

$$\frac{ds}{dt} = 0,$$

$$\frac{dq}{dt} = 0.$$

Rearranging the system of steady state equations gives

$$c(\alpha I + k_f + k_d + k_n s + k_p(1-q)) - I\alpha = 0, \tag{3.1}$$

$$s(\lambda_b c P_C + \lambda_r(1-q)) - \lambda_b c P_C = 0, \tag{3.2}$$

$$q(\gamma + c k_p \frac{P_C}{P_Q}) - c k_p(\frac{P_C}{P_Q}) = 0. \tag{3.3}$$

This is a nonlinear system of equations.

3.1 Descartes rule of signs

Descartes rule of signs is a method of determining the maximum number of positive and negative real roots of a polynomial [8]. It says that the number of positive real zeroes of a polynomial function f(x) is the same or less than by an even numbers as the number of changes in the signs of the coefficients [8]. It also states that number of negative real zeroes of f(x) is the same as the number of changes in sign of the coefficients of the terms of f(-x) or less than this by an even number [8].

Before we apply the Descartes rule of signs in our nonlinear ODEs, we have to write the equations as polynomial functions. To do that, we uses the equations (3.1), (3.2) and (3.3)

$$c(\alpha I + k_f + k_d + k_n s + k_p(1-q)) - I\alpha = 0, \tag{3.4}$$

$$s(\lambda_b c P_C + \lambda_r(1-q)) - \lambda_b c P_C = 0, \tag{3.5}$$

$$q(\gamma + c k_p \frac{P_C}{P_Q}) - c k_p(\frac{P_C}{P_Q}) = 0. \tag{3.6}$$

Rearranging the equation (3.4) and (3.5) gives

$$c = \frac{\alpha\ I}{(\alpha I + k_f + k_d + k_n s + k_p(1-q))} \tag{3.7}$$

and

$$\lambda_b P_C\ c(1-s) = \lambda_r(1-q)\ s. \tag{3.8}$$

From equation (3.6), we again rearrange the equation for c to get

$$c = \frac{\gamma\ q\ P_Q}{k_p(1-q)\ P_C}. \tag{3.9}$$

Now, we substitute c from (3.9) into (3.8) to get expression for s

$$\frac{\lambda_b\ P_C\ \gamma\ q\ P_Q}{k_p(1-q)\ P_C}(1-s) = \lambda_r(1-q)s$$

and rearranging the equation for s gives

$$s = \frac{\lambda_b\ \gamma\ q\ P_Q}{\lambda_b\ \gamma\ q\ P_Q + k_p(1-q)^2\lambda_r}. \tag{3.10}$$

Substituting the expressions s from (3.10) and c from (3.9) into (3.7) we get,

$$\frac{\gamma\ q\ P_Q}{k_p(1-q)\ P_C} = \frac{\alpha\ I}{(\alpha I + k_f + k_d + k_n \frac{\lambda_b\ \gamma\ q\ P_Q}{\lambda_b\ \gamma\ q\ P_Q + k_p(1-q)^2\lambda_r} + k_p(1-q))}$$

Multiply both the numerator and denominator by $\lambda_b\ \gamma\ q\ P_Q + k_p(1-q)^2\lambda_r$ and then doing cross multiplying gives

$$[(\alpha I + k_f + k_d + k_p(1-q))(\lambda_b\gamma q P_Q + k_p\lambda_r(1-q)^2) + k_n\lambda_b\gamma q P_Q](\gamma q P_Q) = I\alpha(\lambda_b\gamma q P_Q + k_p\lambda_r(1-q)^2)(k_p(1-q)P_C).$$

Now, collecting powers of q and combining all parameters into single parameters for each term gives

$$(q) = A\ q^4 + B\ q^3 + C\ q^2 + D\ q + E = 0 \tag{3.11}$$

where,

$A = -k_p^2 P_Q \gamma \lambda_r,$

$B = -k_p^2 P_Q^2 \gamma^2 \lambda_b + I k_p^2 P_C \alpha \lambda_r + \alpha I k_p P_Q \gamma \lambda_r + k_d k_p P_Q \gamma \lambda_r + k_f k_p P_Q \gamma \lambda_r + 3k_p^2 P_Q \gamma \lambda_r,$

$C = I k_p P_C P_Q \alpha \gamma \lambda_b + \alpha I P_Q^2 \gamma^2 \lambda_b + k_d P_Q^2 \gamma^2 \lambda_b + k_f P_Q^2 \gamma^2 \lambda_b + k_n P_Q^2 \gamma^2 \lambda_b + k_p P_Q^2 \gamma^2 \lambda_b - 3 I k_p^2 P_C \alpha \lambda_r - 2k_d k_p P_Q \gamma \lambda_r - 2k_f k_p P_Q \gamma \lambda_r - 3k_p^2 P_Q \gamma \lambda_r,$

$D = -I k_p P_C P_Q \alpha \gamma \lambda_b + 3 I k_p^2 P_C \alpha \lambda_r + \alpha I k_p P_Q \gamma \lambda_r + k_d k_p P_Q \gamma \lambda_r + k_f k_p P_Q \gamma \lambda_r + k_p^2 P_Q \gamma \lambda_r,$

$E = -I k_p^2 P_C \alpha \lambda_r.$

Assuming all the parameters and pool values are positive and comparing the magnitude of all parameters and pool values from table (2.2) and (2.3), then that will gives

A is Negative, B is Positive, C is Negative, D is Positive and E is Negative.

Since A, C and E are negatives, the sign of coefficients of equation (3.11) is changes to

$$(q) = -A\ q^4 + B\ q^3 - C\ q^2 + D\ q - E \tag{3.12}$$

Using Descartes rule of signs for positive polynomial function,

$$f(q) = -A\ q^4 + B\ q^3 - C\ q^2 + D\ q - E$$

Total changes of sign = 4. So, it will have 4 positive maximum roots.
Other possible roots: $4 - 2 = 2$ and $2 - 2 = 0$.
Therefore, there will be 4 or 2 or 0 positive roots.
Similarly for negative (q) we have,

$$-A\ q^4 - B\ q^3 - C\ q^2 - D\ q - E$$

so 0 sign of changes. It means there are no negative roots.

Now, we want to know the positive roots if $q < 1$. Using equations (2.5) and (2.10) gives $Q = 1-q$ and we can rearrange to make $q = 1 - Q$. We substitute q into (3.12) to get in terms of Q and write as polynomial function

$$f(Q) = -A\ Q^4 - (B-4A)\ Q^3 - (6A+C-3)C\ Q^2 - (3B+D-4A+2C)\ Q + (B+D+C-A-E)Q^0$$

Using the Descartes rule of signs, it gives 1 sign change. So, only one positive root of Q.
Now, for negative Q it gives,

$$f(-Q) = -A\ Q^4 + (B-4A)\ Q^3 - (6A+C-3)C\ Q^2 + (3B+D-4A+2C)\ Q + (B+D+C-A-E)Q^0.$$

3 change of signs = 3 maximum negative roots of Q.
Other possible roots: $3 - 2 = 1$
Therefore, there will be 3 or 1 negative roots of Q.

We are interested in the number of positive steady-state roots for q in the interval $0 < q < 1$. The polynomial is a quartic which has 4 total roots but we are only interested in positive roots. From the Descartes rule of signs, q gave 4 maximum positive roots and Q gave only 1 positive root. Since $Q = 1 - q$ and that gives $q = 1 - Q$. We deduce that q has only 1 positive root which is less than 1.
Therefore, q has only 1 positive steady-state which lies between 0 and 1.

Knowing the condition of steady-state for q, we can use to get s and c. From equation 3.10 we have

$$s = \frac{\lambda_b\ \gamma\ q\ P_Q}{\lambda_b\ \gamma\ q\ P_Q + k_p(1-q)^2\lambda_r}.$$

In the above equation of s, if we substitute $q = 0$ then will get $s = 0$ and if $q = 1$ then $s = 1$. Assuming all the parameters and pool values are positive, if we substitute q lies between 0 and 1 in the equation (3.10) then s will also lies between 0 and 1.

From equation 3.9 we have

$$c = \frac{\gamma\ q\ P_Q}{k_p(1-q)\ P_C}.$$

If we substitute $q = 0$ into the above equation of (c), we will get $c = 0$ and q can not equal to 1. From the table (2.2) and (2.3) we have,

$$\text{magnitude of } P_Q \approx \text{magnitude of } P_C$$

and

$$\text{magnitude of } k_p > \text{magnitude of } \gamma.$$

Depending upon the magnitude of parameters and pool values above, if we substitute q which lies between 0 and 1 in the equation (3.9) then c will also lies between 0 and 1.

We shall seek the steady state by the Newton-Raphson method.

3.2 Newton-Raphson Method

The Newton-Raphson method is a method of approximating a root x of an equation $f(x) = 0$. We take an initial guess for the root we are trying to find, and we call this initial guess x_0. [7] To implement it analytically we need a formula for each approximation in terms of the previous one, i.e. we need x_{n+1} in terms of x_n where x_{n+1} denotes the next iteration and x_n denotes previous iteration, i.e.

$$x_{n+1} = x_n - \frac{f(x_n)}{f'(x_n)}$$

Here, we used the multivariate Newton-Raphson method on our steady-state equations (3.1), (3.2) and (3.3), which involves the Jacobian matrix

$$J(\vec{x_n}) = \begin{pmatrix} \frac{df}{dc} & \frac{df}{ds} & \frac{df}{dq} \\ \frac{dg}{dc} & \frac{dg}{ds} & \frac{dg}{dq} \\ \frac{dh}{dc} & \frac{dh}{ds} & \frac{dh}{dq} \end{pmatrix}.$$

$$\text{Let } \vec{x}_n = \begin{bmatrix} \mathrm{c}_n \\ \mathrm{s}_n \\ \mathrm{q}_n \end{bmatrix} \text{ and } \vec{F_n} = \begin{pmatrix} \mathrm{f}(\mathrm{c}_n, s_n, q_n) \\ \mathrm{g}(\mathrm{c}_n, s_n, q_n) \\ \mathrm{h}(\mathrm{c}_n, s_n, q_n) \end{pmatrix}.$$

where

$$f(c_n, s_n, q_n) = c_n(\alpha I + k_f + k_d + k_n \times s_n + k_p \times (1 - q_n)) - I\alpha$$

$$g(c_n, s_n, q_n) = s_n(\lambda_b c_n P_C + \lambda_r(1 - q_n)) - \lambda_b c_n P_C$$

$$h(c_n, s_n, q_n) = q_n(\gamma + c_n k_p \frac{P_C}{P_Q}) - (c_n k_p (\frac{P_C}{P_Q})$$

We find the partial derivatives in terms of c, s and q and Jacobian matrix is

$$J(\vec{x_n}) = \begin{pmatrix} \alpha I + k_f + k_d + k_n s_n + k_p(1 - p_n) & k_n c_n & -k_p c_n \\ \lambda_b P_C(s_n - 1) & \lambda_b c_n P_C + \lambda_r(1 - q_n) & -\lambda_r s_n \\ \frac{(k_p P_C(q_n - 1))}{P_Q} & 0 & \gamma + \frac{(k_p P_C c_n)}{P_Q} \end{pmatrix}.$$

Let's search estimates for c, s and q with initial guess

$$\vec{x}_0 = \begin{bmatrix} c_0 \\ s_0 \\ q_0 \end{bmatrix} = \begin{bmatrix} 0.5 \\ 0.36 \\ 0.82 \end{bmatrix}.$$

Using the initial guess and values of parameters from tables (2.2) and (2.3) then we have

$$\vec{F_0} = \begin{pmatrix} f(c_0, s_0, q_0) \\ g(c_0, s_0, q_0) \\ h(c_0, s_0, q_0) \end{pmatrix} = \begin{pmatrix} 1.6 \times 10^9 \\ -8.4 \times 10^9 \\ -4648571426 \end{pmatrix}.$$

Applying the Newton-Raphson method

$$\vec{x_{n+1}} = \vec{x_n} - J^{-1}(\vec{x_n})\vec{F_n}$$

where $\vec{x_{n+1}}$ denotes values for (c, s, q) at the next iteration and $\vec{x_n}$ denotes previous values for (c, s, q). Both $\vec{x_{n+1}}$ and $\vec{x_n}$ are in vector form of $[c_n, s_n, q_n]$. $J^{-1}(\vec{x_n})$ is the inverse matrix of the Jacobian. In the first iteration, we have

$$\vec{x_1} = \vec{x_0} - J^{-1}(\vec{x})\vec{F_0}$$

then the process continue until it converges.

The convergence criterion used to terminate the iteration was as follows

$$\left\| \vec{x^{n+1}} - \vec{x^n} \right\| \leq TOL$$

iter= 0	$c = 0.000000017184656$	$s = 0.359999980534294$	$q = 0.820000006099454$
iter= 1	$c = 0.000000005156733$	$s = 0.205933723422758$	$q = 0.871323557731450$
iter= 2	$c = 0.000000001982175$	$s = 0.113910677804177$	$q = 0.911406711094306$
iter= 3	$c = 0.000000001293512$	$s = 0.084350855341095$	$q = 0.943951007104135$
iter= 4	$c = 0.000000001227552$	$s = 0.083650493708679$	$q = 0.957849278503740$
iter= 5	$c = 0.000000001224451$	$s = 0.084358982860184$	$q = 0.958463056124308$
iter= 6	$c = 0.000000001224423$	$s = 0.084367992393470$	$q = 0.958463625458527$
iter= 7	$c = 0.000000001224423$	$s = 0.084367992564821$	$q = 0.958463625475680$

Table 3.1: Steady-states of 3 ODEs for c, s and q.

where TOL is a very small positive constant. We chose $TOL = 10^{-9}$ and Newton Raphson method was applied until a steady state was achieved. We present numerical results which are summarised in Table 3.1.
Table 3.1 shows the steady-states of c, s and q using Newton-Raphson method which are positive and between 0 and 1. Seven iterations were required to converge within the tolerance to get steady-states for c, s and q up to 7 significant figure. We see that c converges very quickly compared to s and q, showing that the initial guess is a good one.

Descartes rule of signs shows that the root obtained by Newton-Raphson method is the only one positive root which lies between 0 and 1. Now, we are interested to know are these steady-states values stable in the system of 3 ODEs?

In the next section we look at the stability of the steady states of 3 ODEs.

3.3 Stability of steady states

Using the equations (2.11), (2.12) and (2.13), we have system of 3 nonlinear ODEs which are given by

$$\frac{dc}{dt} = \alpha I(1-c) + c(-k_f - k_d - k_n s - k_p(1-q)). \tag{3.13}$$

$$\frac{ds}{dt} = \lambda_b P_C \ c(1-s) - \lambda_r(1-q) \ s. \tag{3.14}$$

$$\frac{dq}{dt} = k_p(1-q)\frac{P_C}{P_Q} \ c - \gamma \ q. \tag{3.15}$$

We have already determined the steady state values of c, s, q which we call $\overline{c}$, $\overline{s}$ and $\overline{q}$. We now proceed to explore the stability of this solution by considering the perturbation

$$c = \overline{c} + \delta, \ s = \overline{s} + \sigma, \ q = \overline{q} + \beta \tag{3.16}$$

where δ, σ and β are small quantities termed *perturbations* of the steady-states $\overline{c}$, $\overline{s}$ and $\overline{q}$ respectively.
Now we substitute 3.16) into (3.13), (3.14) and (3.15) to get,

$$\frac{d\overline{c}}{dt} + \frac{d\delta}{dt} = \alpha I + (\overline{c} + \delta)(-\alpha I - k_f - k_d - k_n(\overline{s} + \sigma) - k_p(1 - (\overline{q} + \beta)))$$

$$\frac{d\bar{s}}{dt} + \frac{d\sigma}{dt} = \lambda_b P_C(\bar{c}+\delta)(1-(\bar{s}+\sigma)) - \lambda_r(1-(\bar{q}+\beta))(\bar{s}+\sigma)$$

$$\frac{d\bar{q}}{dt} + \frac{d\beta}{dt} = k_p(1-(\bar{q}+\beta))\frac{P_C}{P_Q}(\bar{c}+\delta) - \gamma(\bar{q}+\beta)$$

and keeping only first powers of δ, σ and β gives:

$$\frac{d\delta}{dt} = (-\alpha I - k_f - k_d - k_n\bar{s} - k_p(1-\bar{q}))\ \delta - k_n\bar{c}\ \sigma + k_p\bar{c}\ \beta. \tag{3.17}$$

$$\frac{d\sigma}{dt} = (\lambda_b P_C - \lambda_b P_C\bar{s})\ \delta + (\lambda_r(1-\bar{q}) - \lambda_b P_C\bar{c})\ \sigma + \lambda_r\bar{s}\ \beta. \tag{3.18}$$

$$\frac{d\beta}{dt} = (k_p\frac{P_C}{P_Q} - k_p\frac{P_C}{P_Q}\bar{q})\ \delta - \frac{P_C}{P_Q}\bar{c}k_p\ \beta. \tag{3.19}$$

Writing the equations (3.17), (3.18) and (3.19) in matrix form we get,

$$\frac{d}{dt}\begin{pmatrix}\delta\\ \sigma\\ \beta\end{pmatrix} = \begin{bmatrix} \text{-}\alpha I - k_f - k_d - k_n\bar{s} - k_p(1-\bar{q}) & \text{-k}_n\bar{c} & \text{k}_p\bar{c} \\ \lambda_b P_C - \lambda_b P_C\bar{s} & \lambda_r(1-\bar{q} - \lambda_b P_C\bar{c} & \lambda_r\bar{s} \\ \text{k}_p\frac{P_C}{P_Q} - k_p\frac{P_C}{P_Q}\bar{q} & 0 & \text{-}\ \bar{c}k_p\frac{P_C}{P_Q} \end{bmatrix} \begin{bmatrix}\delta\\ \sigma\\ \beta\end{bmatrix}$$

By substituting the numerical values of the steady-states of $\bar{c}$, $\bar{s}$ and $\bar{q}$, we get the eigenvalues of the matrix

$$-1.124\times 10^9,\ -48.578+23.653i,\ -48.578-23.653i$$

We are only interested in real parts which are all negative, hence the steady-state is stable.

Chapter 4

ODE solver for 3 ODEs model

Before we use an ODE solver to solve the systems of 3 nonlinear ODEs, we want to know the stiffness of the system, which is presented in the following section.

4.1 Stiffness of 3 ODEs

We need to find the condition number of Jacobian at the initial time to know the initial stiffness of the system. The 3 nonlinear ODEs are

$$\frac{dc}{dt} = \alpha I(1-c) + c(-k_f - k_d - k_n s - k_p(1-q)).$$

$$\frac{ds}{dt} = \lambda_b P_C \ c(1-s) - \lambda_r(1-q) \ s.$$

$$\frac{dq}{dt} = k_p(1-q)\frac{P_C}{P_Q} \ c - \gamma \ q.$$

Setting

$$\frac{dc}{dt} = f(c,s,q), \ \frac{ds}{dt} = g(c,s,q), \frac{dg}{dt} = h(c,s,q)$$

we get

$$f(c,s,q) = \alpha I(1-c) + c(-k_f - k_d - k_n s - k_p(1-q)).$$

$$g(c,s,q) = \lambda_b P_C \ c(1-s) - \lambda_r(1-q) \ s.$$

$$h(c,s,q) = k_p(1-q)\frac{P_C}{P_Q} \ c - \gamma \ q.$$

We now get partial derivatives of $f(c,s,q)$, $g(c,sq)$ and $h(c,s,q)$ in terms of c, s and q and obtain the Jacobian matrix form :

$$J = \begin{pmatrix} \frac{df}{dc} & \frac{df}{ds} & \frac{df}{dq} \\ \frac{dg}{dc} & \frac{dg}{ds} & \frac{dg}{dq} \\ \frac{dh}{dc} & \frac{dh}{ds} & \frac{dh}{dq} \end{pmatrix}.$$

$$J = \begin{pmatrix} -\alpha I - k_f - k_d - k_n s - k_p(1-q) & -k_n c & k_p c \\ \lambda_b P_C(1-s) & \lambda_b P_C \ c - \lambda_r(1-q) & \lambda_r s \\ k_p(1-q)\frac{P_C}{P_Q} & 0 & -k_p(1-q)\frac{P_C}{P_Q} c - \gamma \end{pmatrix}.$$

Substituting the initial conditions of $c = 0.0$, $s = 0.02$ and $q = 0.0$ at time $= 0$ and the numerical values of parameters and pool values from table (2.2) and (2.3) into Jacobian matrix (J) we get

$$cond(J) \approx 10^{12}$$

where $cond(J)$ is $\frac{max|\lambda_J|}{min|\lambda_J|}$.
Hence the system of 3 ODEs is extremely stiff.

In the next section, we used an integration package to get the results for the system of 3 nonlinear ODEs.

4.2 Results of 3 ODEs solved using $ode23s$

This section is about a numerical solution of the system of 3 ODEs solved by using the stiff ODE solver $ode23s$ of MATLAB. Before using the solver, we discuss briefly about $ode23s$ and its useful features for stiff systems.

The ODE solver $ode23s$ is based on the Runge-Kutta scheme $2nd$ and $3rd$ order and the 's' signifies that it is stiff solver [9] [14]. First order ODEs are solved numerically using many different integration routines. Among the most popular methods are Runge-Kutta methods. Of course, very few nonlinear systems can be solved explicitly and basic methods to solve them begin with the simple Explicit Euler scheme, but Runge-Kutta schemes are more stable and accurate than the Euler method [6]. Another ODE solver $ode45$ [11] [14](based on higher order explicit Runge-Kutta schemes) is also efficient but may become unstable with stiff systems. Therefore, $ode23s$ is used for our stiff problem which can be made more efficient by using crude tolerance to solve the stiff systems [10] [14]. The $ode23s$ solver chooses efficient time steps to get better solutions. Hence, it is well adapted for the stiff problem.

Now, we used $ode23s$ to solve the systems of 3 ODEs to see the behaviour of c by choosing different tolerance to determine the behaviour of the solution at small time with the initial conditions $c = 0.0$, $s = 0.02$ and $q = 0.0$.

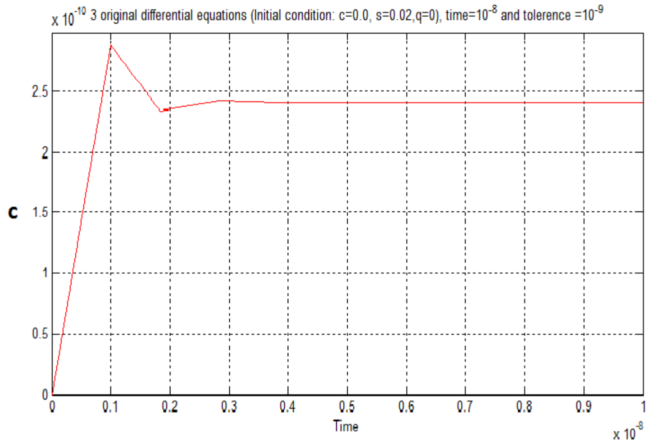

Figure 4.1: System of 3 ODEs for c with a final time $=10^{-8}$ and tolerance$=\ 10^{-9}$.

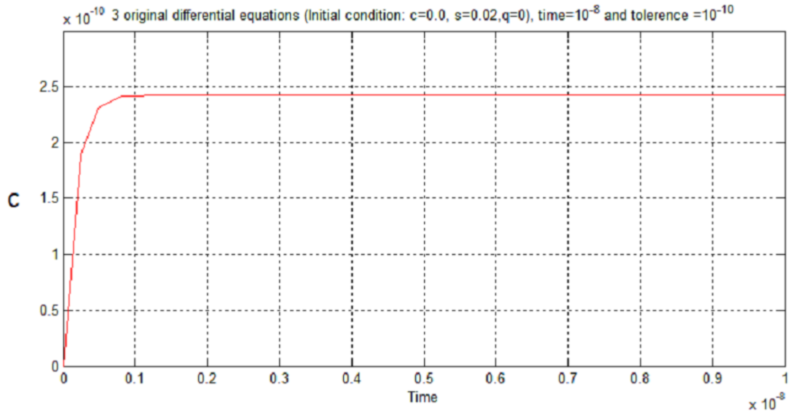

Figure 4.2: System of 3 ODEs for c with a final time $=10^{-8}$ and tolerance$=\ 10^{-10}$.

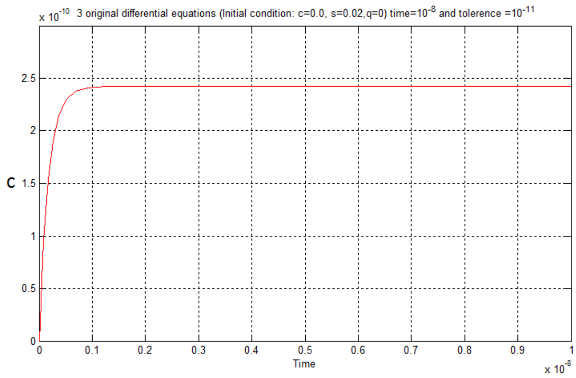

Figure 4.3: System of 3 ODEs for c with a final time $=10^{-8}$ and tolerance= 10^{-11}.

Figures (4.1), (4.2) and (4.3) represent the initial state behaviour of c up to the very small time $=1 \times 10^{-8}$ with different tolerances. We have used RelTol $=10^{-11}$ and AbsTol$=10^{-11}$. RelTol is the relative accuracy tolerance, a measure of the error relative to the size of each solution component [9]. AbsTol is a scalar or vector of the absolute error tolerances determine the accuracy when the solution approaches zero [9].

Comparing the three figures (4.1), (4.2) and (4.3), there is some change in behaviour of c and as tolerance gets to 10^{-11} it gives a much smoother graph which is the best one. We plot the number of time steps it uses for the figure (4.3).

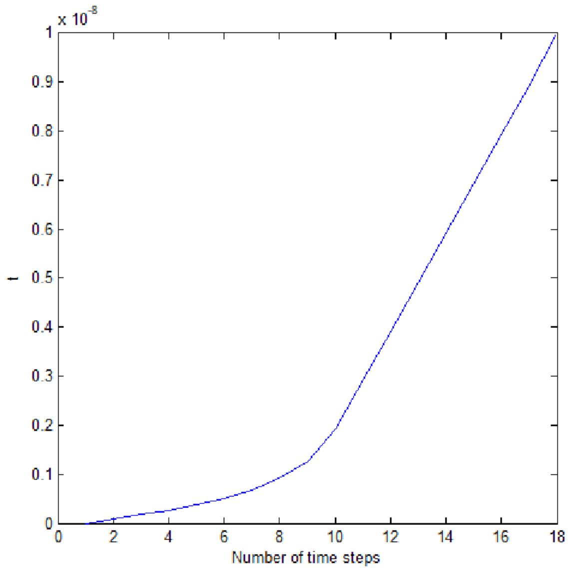

Figure 4.4: Number of time step used for initial behaviour of c.

In figure 4.4 we plot the time against the number of time steps, showing that the time intervals start very small and then increase to a fixed interval.

We have seen the short term behaviour of c which can be changed by using different tolerances. The smaller the tolerance the better the plots of c since the 3 ODEs model is a very stiff system. Now, we want to find the steady solution of 3 ODEs for c, s and q by using the best tolerance $= 10^{-11}$ and final time =0.25.

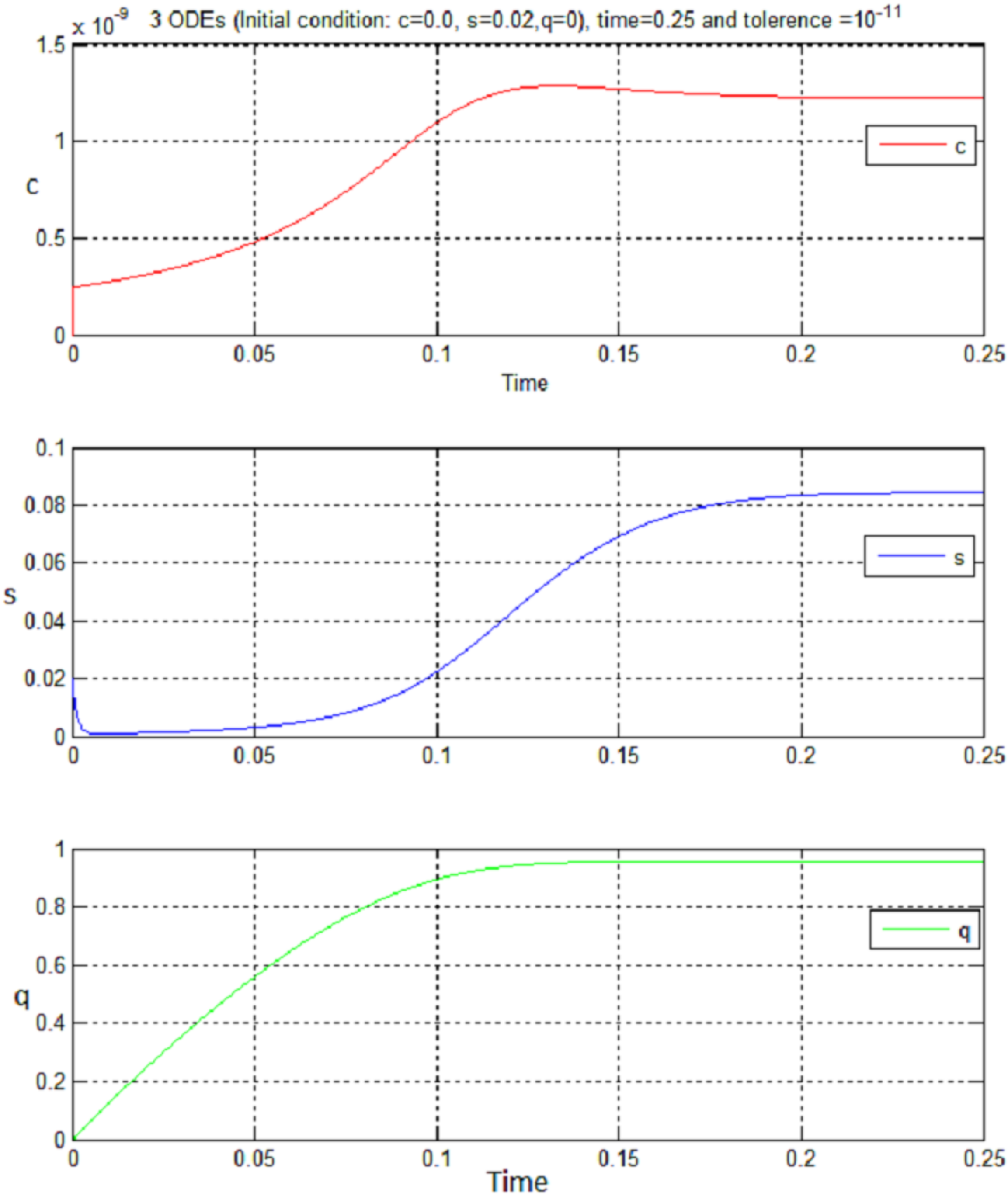

Figure 4.5: System of 3 ODEs for c, s and q with a final time =0.25 and tolerance= 10^{-11}.

Figures $4.1 - 4.3$ shows that around t=1×10^{-8} the graph of c becomes almost constant. Figure (4.4) shows that c progresses rapidly whereas s and q show only small changes. Around time =0.2, the graphs of c, s and q starts to becomes steady solutions. Their final steady-states values of $c = 1.22 \times 10^{-9}$, $s = 0.084$ and $q = 0.96$ are same as the steady-states of c, s and q (see table 3.1) which were calculated using the Newton-Raphson method.

Now, since c changes very quickly for very small times the system of 3 ODEs can be reduced to a system of 2 ODEs, as described in the model [1].

In next chapter, we will find the steady state and stability of the 2 ODEs system and we expect them to be same as 3 ODEs. And we also look at the stiffness of 2 ODEs system which is expected to be less stiff than that of the 3 ODEs.

Chapter 5

Two ODEs model

5.1 Steady states and stability

In this chapter, we begin by reducing the systems of 3 ODEs to a systems of 2 ODEs. We have seen that equation (2.11) presents a very fast process and is therefore can be set to zero after a short time. Rearranging the equation with $\frac{dc}{dt} = 0$ for c gives

$$c = \frac{\alpha\ I}{(\alpha I + k_f + k_d + k_n s + k_p(1-q))}. \tag{5.1}$$

The two remaining equations of the 3 ODEs system are the same as equations (2.12) and (2.13) and they are

$$\frac{ds}{dt} = \lambda_b P_C\ c(1-s) - \lambda_r(1-q)\ s \tag{5.2}$$

$$\frac{dq}{dt} = k_p(1-q)\frac{P_C}{P_Q}\ c - \gamma\ q \tag{5.3}$$

which do not progress so rapidly. We substitute c from (5.1) into above (5.2) and (5.3) to get

$$\frac{ds}{dt} = \frac{\alpha I \lambda_b P_C\ (1-s)}{(\alpha I + k_f + k_d + k_n s + k_p(1-q))} - \lambda_r(1-q)\ s \tag{5.4}$$

$$\frac{dq}{dt} = \frac{k_p(1-q)P_C \alpha I}{P_Q(\alpha I + k_f + k_d + k_n s + k_p(1-q))} - \gamma\ q. \tag{5.5}$$

Now, we have system of 2 ODEs in terms of s and q.
The steady-states of the system of 2 ODEs are given by

$$\frac{ds}{dt} = 0,$$

$$\frac{dq}{dt} = 0.$$

Rearranging the states state equations (5.4) and (5.5) gives

$$\alpha I \lambda_b P_C\ (1-s) - \lambda_r(1-q)\ s(\alpha I + k_f + k_d + k_n s + k_p(1-q)) = 0 \tag{5.6}$$

$$k_p(1-q)P_C \alpha I - \gamma\ q P_Q(\alpha I + k_f + k_d + k_n s + k_p(1-q)) = 0. \tag{5.7}$$

Similarly, as in the system of 3 ODEs, the Descartes rule of signs tell us there is a unique steady states of c, s and q which is positive and lies between 0 and 1 for the system of 2 ODEs.

We used the Newton-Raphson method in equations (5.6) and (5.7), which involves the Jacobian matrix

$$J(\vec{x_n}) = \begin{pmatrix} \frac{df}{ds} & \frac{df}{dq} \\ \frac{dg}{ds} & \frac{dg}{dq} \end{pmatrix}.$$

$$\text{Let } \vec{x}_n = \begin{bmatrix} \mathrm{s}_n \\ \mathrm{q}_n \end{bmatrix} \text{ and } F_n = \begin{pmatrix} \mathrm{f}(\mathrm{s}_n, q_n) \\ \mathrm{g}(\mathrm{s}_n, q_n) \end{pmatrix}.$$

where,

$$f(s_n, q_n) = \alpha I \lambda_b P_C \ (1-s) - \lambda_r (1-q) \ s(\alpha I + k_f + k_d + k_n s + k_p(1-q))$$

$$g(s_n, q_n) = k_p(1-q) P_C \alpha I - \gamma \ q P_Q(\alpha I + k_f + k_d + k_n s + k_p(1-q))$$

We find the partial derivatives in terms of s and q and Jacobian matrix gives

$$J(\vec{x_n}) = \begin{pmatrix} -\alpha I \lambda_b P_C - \lambda_r(1-q)(\alpha I + k_f + k_d + 2 s_n k_n + k_p(1-q_n)) & \lambda_r s_n(\alpha I + k_f + k_d + k_n s_n + 2k_p) - 2 q_n \lambda_r s_n k_p \\ -\gamma q_n P_Q k_n & -k_p P_C \alpha I - \gamma P_Q(\alpha I + k_f + k_d + k_n s_n + k_p(1-2q_n)) \end{pmatrix}.$$

Using the initial guess

$$\vec{x}_0 = \begin{bmatrix} s_0 \\ q_0 \end{bmatrix} = \begin{bmatrix} 0.36 \\ 0.82 \end{bmatrix}.$$

and applying the Newton-Raphson method

$$x_{n+1} = x_n - J^{-1}(\vec{x_n}) F_n$$

we find the steady state of s and q until it convergence criterion as follows

$$\left\| x^{n+1} - x^n \right\| \leq TOL$$

where x_{n+1} denotes values for (s, q) at the next iterations and x_n denotes previous values for (s, q). Both x_{n+1} and x_n are in vector form of $[s_n, q_n]$. $J^{-1}(\vec{x_n})$ is the inverse matrix of Jacobian. We chose $TOL = 10^{-9}$ and the steady-stated were achieved which is presented in table (5.1)

iter= 0	$s = 0.313468877469675$	$q = 0.927582881509019$
iter= 1	$s = 0.181643421532470$	$q = 0.946035293381273$
iter= 2	$s = 0.110221215678293$	$q = 0.955124453638258$
iter= 3	$s = 0.086899725790324$	$q = 0.958134328718685$
iter= 4	$s = 0.084395758589826$	$q = 0.958460005149877$
iter= 5	$s = 0.084367996112138$	$q = 0.958463625072840$
iter= 6	$s = 0.084367992616843$	$q = 0.958463625413674$
iter= 7	$s = 0.084367992564843$	$q = 0.958463625475684$

Table 5.1: Steady-states of 2 ODEs for s and q.

Table (5.1) shows the positive steady-state of s and q and we substitute the values of s and q from the final iteration into equation (5.1)

$$c = \frac{\alpha \ I}{(\alpha I + k_f + k_d + k_n s + k_p(1-q))}$$

to get $c = 0.000000001224403$. We have the same steady-states of c, s and q as in the 3 ODEs and also Descartes rule of sign already proves that these steady states have only one positive root which lies between 0 and 1.

Now, we consider the stability of the steady state solutions. We already knew about the equation (2.15) progressing very rapidly and the system of 3 equations can be reduced into system of 2 equations. From equations (5.4) and (5.5) we have the systems of 2 ODEs

$$\frac{ds}{dt} = \frac{\alpha I \lambda_b P_C\ (1-s)}{(\alpha I + k_f + k_d + k_n s + k_p(1-q))} - \lambda_r(1-q)\ s \tag{5.8}$$

$$\frac{dq}{dt} = \frac{k_p(1-q)P_C \alpha I}{P_Q(\alpha I + k_f + k_d + k_n s + k_p(1-q))} - \gamma\ q. \tag{5.9}$$

To find stability we write

$$s = \overline{s} + \sigma,\ \ q = \overline{q} + \beta \tag{5.10}$$

where $\overline{s}$ and $\overline{q}$ are the steady states of s and q respectively and then substitute (5.10) into (5.8) and (5.9) just keeping first powers of σ and β only gives

$$\frac{d\sigma}{dt} = (\lambda_r(\overline{q}-1)\ \sigma + \lambda_r \overline{s}\ \beta. \tag{5.11}$$

$$\frac{d\beta}{dt} = \gamma\beta. \tag{5.12}$$

Writing equations (5.11) and (5.12) in matrix form

$$\begin{bmatrix} \lambda_r(\overline{q}-1) & \lambda_r\overline{s} \\ 0 & \gamma \end{bmatrix} \begin{bmatrix} \sigma \\ \beta \end{bmatrix} = 0$$

$$(\lambda_r(\overline{q}-1) - \lambda)(-\gamma - \lambda) = 0$$

and the eigenvalues are given by $\lambda_1 = \lambda_r(\overline{q}-1)$ and $\lambda_2 = -\gamma$.

Since, steady-state of $\overline{q}$ is less than 1 which we already verified in the results of Newton Raphson method and gamma is positive parameter from table (2.2).

So, we get $\lambda_{1,2} < 0$. Therefore, the steady state is stable.

We found out the stability of steady-state is stable for both systems of 2 and 3 nonlinear ODEs. For system of 2 nonlinear ODEs, stability condition was verified without substituting the numerical values to identify the eigenvalues.

In the next section, we will find about the stiffness of system of 2 ODEs by finding the condition number of Jacobian at initial time.

5.2 Stiffness of 2 ODEs and use of integration packages

Considering the system of 2 nonlinear ODEs we have

$$\frac{ds}{dt} = \frac{\alpha I \lambda_b P_C(1-s)}{(\alpha I + k_f + k_d + k_n s + k_p(1-q))} - \lambda_r(1-q)\ s,$$

$$\frac{dq}{dt} = \frac{k_p(1-q)P_C\alpha I}{P_Q(\alpha I + k_f + k_d + k_n s + k_p(1-q))} - \gamma\ q.$$

Let $\frac{ds}{dt} = g(s,q)$, $\frac{dq}{dt} = h(s,q)$ and we write as

$$g(s,q) = \frac{\alpha I \lambda_b P_C\ (1-s)}{(\alpha I + k_f + k_d + k_n s + k_p(1-q))} - \lambda_r(1-q)\ s,$$

$$h(s,q) = \frac{k_p(1-q)P_C\alpha I}{P_Q(\alpha I + k_f + k_d + k_n s + k_p(1-q))} - \gamma\ q.$$

Now writing the partial derivatives in terms of s and q into Jacobian matrix form

$$J = \begin{pmatrix} \frac{dg}{ds} & \frac{dg}{dq} \\ \frac{dh}{ds} & \frac{dh}{dq} \end{pmatrix}.$$

$$J = \begin{pmatrix} \frac{-I\lambda_b\alpha P_C}{(\alpha I+k_f+k_d+k_n s+k_p(1-q))} - \frac{I\lambda_b\alpha P_C(1-s)k_n}{(\alpha I+k_f+k_d+k_n s+k_p(1-q))^2} - \lambda_r(1-q) & \frac{I\lambda_b\alpha P_C(1-s)k_p}{(\alpha I+k_f+k_d+k_n\ s+k_p(1-q))^2} + \lambda_r s \\ \frac{-Ik_p(1-q)P_C\alpha k_n}{(P_Q(\alpha I+k_f+k_d+k_n s+k_p(1-q))^2} & \frac{-Ik_pP_C\alpha P_Q(\alpha I+k_f+k_d+k_n s+k_p(1-q))+Ik_p^2(1-q)P_C\alpha}{P_Q^2(\alpha I+k_f+k_d+k_n s+k_p(1-q))^2} - \gamma \end{pmatrix}$$

Substituting the numerical values of parameters and pool values from table (2.2) and (2.3) into Jacobian matrix (J) with the initial conditions of $s = 0.02$ and $q = 0.0$ at time $= 0$, we get

$$cond(J) = 54.342$$

From 3 ODEs we have $cond(J) \approx 10^{12}$ and $cond(J) \approx 54$ from 2 ODEs. Thus, the system of 3 ODEs is more stiff than the system of 2 ODEs.

After finding the condition number of the Jacobian for the system of 2 ODEs, we still need to use a stiff solver $ode23s$ to solve the system of 2 ODEs even though it is less stiff compared to 3 ODEs.

Now, we use the $ode23s$ to solve the systems of 2 nonlinear ODEs. For the systems of 2 ODEs, we should only plot the graphs of s and q but by substituting s and q into

$$c = \frac{\alpha\ I}{(\alpha I + k_f + k_d + k_n s + k_p(1-q))}.$$

we plot c to see the behaviour of c and also to find steady state value of c.

We have used the initial conditions $s = 0.02$ and $q = 0.0$ and can choose tolerance $=10^{-4}$ because it is less stiff than 3 ODEs and get the following graph

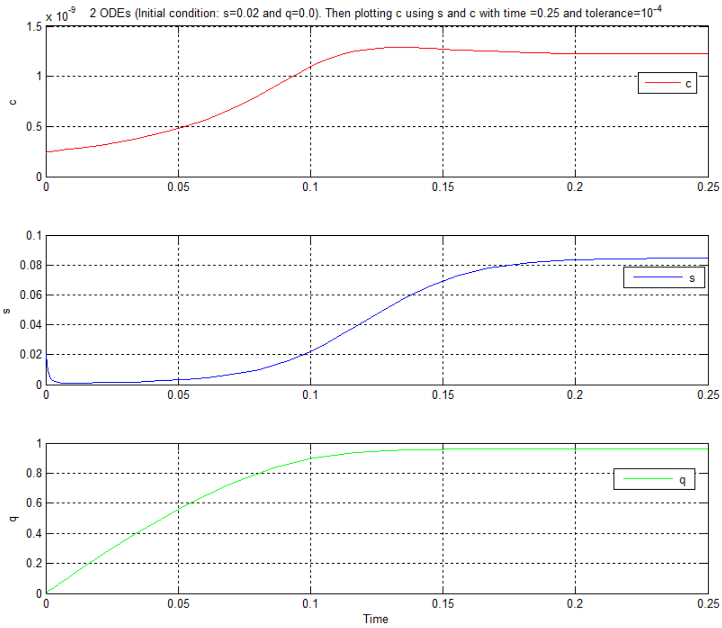

Figure 5.1: System of 2 ODEs for s and q and then plotting c using s and q with using a final time =0.6 and tolerance= 10^{-4}.

In the figure (5.1) shows that c is not progresses rapidly as in the figure (4.5) of 3 ODEs. Here, c initially starts from 0.25×10^{-9} as using initial values of s and q. The final steady state values of c, s and q are all same as in figure (4.1) of 3 ODEs which also matches the steady states of c, s and q calculated by using the Newton-Raphson method.

Now, unlike system of 3 ODEs c does not change very quickly for small times. Therefore, the behaviour of c at very small time up to 10^{-8} will not give any useful information as the plot of c will give a steady line going diagonally up. So we decided to plot the graphs of s instead using final time =0.01 with tolerance =10^{-4} to check their initial behaviour as this could be reason for 2 ODEs being a stiff system.

Figure (5.2) presents the initial state of figure (5.1) for s which was calculated using a small time $=0.01$ and tolerance $=10^{-4}$. The figure tells us that, it does not look like the behaviour of s is rapidly changing and we conclude that it is still slowly progressing just like in the system of 3 ODEs.

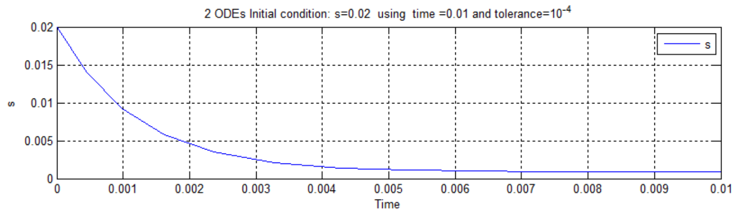

Figure 5.2: System of 2 ODEs for s with a final time $=0.01$ and tolerance$=10^{-4}$.

In the next section, we compared all the results between systems of 3 and 2 ODEs.

5.3 Comparison of results between 3 ODEs and 2 ODEs

Comparing both systems of ODEs, we have got the same steady state solution for c, s and q which are positive and lie between 0 and 1. In addition to that, both systems of ODEs suggest that their steady states are stable. By finding the condition numbers of Jacobian for both systems, 3 ODEs is more stiff than 2 ODEs but 2 ODEs is still stiff. Therefore, we used stiff solver $ode23s$ to solve both systems of ODEs. After using $ode23s$ for both systems, we got the same steady solutions for c, s and q using a final time $=0.25$ and the behaviour of s and q was the same for both.

Now, we are interested in comparing with the figures of 3 and 2 ODEs for c only since s and q process same behaviour for both systems and also starts with same initial condition where as c have different initial conditions. We overplot the graphs of 2 and 3 ODEs for c and we got following graph

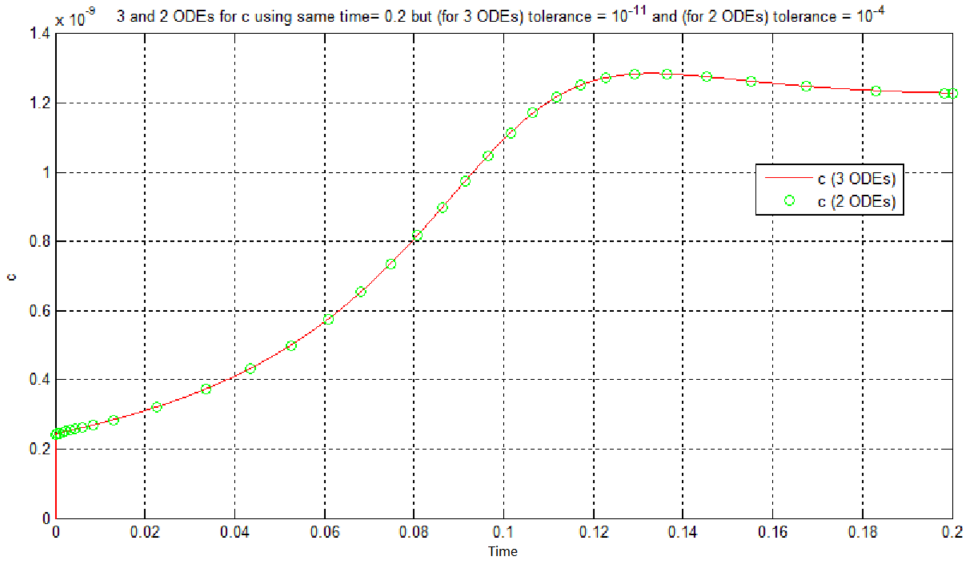

Figure 5.3: Overplots of 3 and 2 ODEs for c using a final time =0.2 but different tolerance 10^{-11} (3 ODEs) and 10^{-4} (2 ODEs).

In the above figure (5.3), the system of 3 for c starts initially from 0 whereas 2 ODEs for c starts from 0.25×10^{-9}. It shows that 3 ODEs for c progresses very rapidly at very small time and starts to behave the same as 2 ODEs from time $= 0.25 \times 10^{-9}$. Although c for 3 ODEs is a line, it is really a large number of individuals values. The c for 2 ODEs shows individual values but in the case of the c for 3 ODEs there are too many values to show individually.

The system of 2 ODEs has a special advantage since it has 2 ODEs which can be solved by using small tolerance $=10^{-4}$ rather than a very much smaller tolerance $=10^{-11}$. Furthermore, asymptotic expansion of 2 ODEs is not necessary require to look at behaviour of c at the initial state.

In next chapter, we look at the asymptotic behaviour of 3 ODEs at small times.

Chapter 6

Asymptotic analysis

We have already dealt with the steady-states, stability and stiffness of the systems of 3 and 2 ODEs in chapter 3, chapter 4 and chapter 5 respectively. Now, we carry out an asymptotic expansion of 3 ODEs and then use ode solver *odes23s* to compare with the numerical results from the system of 3 ODEs which was found in chapter 4. We start with a brief introduction to asymptotic expansions and then approximate the expansions of 3 ODEs close to the initial state.

6.1 Introduction

Many problems do not have exact analytical solutions, often as a result of nonlinearities in the systems [12]. Numerical solution of the equations is one option to represent approximate solutions. However if there are large or small parameters present, the use of perturbation or asymptotic methods can be useful to understand the solution properties [13]. It may be possible to obtain solutions in analytical form, or to reduce the equations to simpler form which can can be solved more easily.
The asymptotic expansion technique is a method to get an approximate solution using asymptotic series. The asymptotic series provides a useful local approximation to the original problem. Suppose we have a differential equation for $u(x;\epsilon)$ which contain a small parameter ϵ. We want to find the solution $u(x;\epsilon)$. In general, we cannot solve the equation exactly. However, supposing we can solve it in the case $\epsilon = 0$, a perturbation method may prove useful in obtaining a solution for small values of ϵ [12]. Thus, we seek a formal solution in the form of a power series in ϵ

$$u(x;\epsilon) = u_0(x) + \epsilon u_1(x) + \epsilon^2 u_2(x) + ...$$

Here $u_0(x)$ is the leading or dominating term, which is the solution of the reduced problem when $\epsilon = 0$ [12]. The series is substituted into the differential equation and boundary condition and the coefficients of like powers of ϵ are equated [12]. This approach will be valid for all sufficiently small ϵ, since powers of ϵ are linearly independent.

In the next section, we apply the method of asymptotic expansions to the system of 3 non-linear ODEs.

6.2 Method of solution and comparison of results with normal 3 ODEs

In this section, we are going to apply the method of asymptotic expansions to the system of 3 non-linear ODEs. The system of 3 nonlinear ODES from equations (3.8), (3.5) and (3.6) is

$$\frac{dc}{dt} = \alpha I(1-c) + c(-k_f - k_d - k_n s - k_p(1-q)),$$

$$\frac{ds}{dt} = \lambda_b P_C \ c(1-s) - \lambda_r(1-q) \ s,$$

$$\frac{dq}{dt} = k_p(1-q)\frac{P_C}{P_Q} \ c - \gamma \ q.$$

Before applying the asymptotic expansion to the above differential equations, we rescale some larger parameters of equations by introducing the very small factor ϵ.
Setting

$$\epsilon \ k_f = K_F$$

$$\epsilon \ k_d = K_D$$

$$\epsilon \ k_n = K_N$$

$$\epsilon \ k_p = K_P$$

$$\epsilon \lambda_b = \Lambda_B$$

and substituting the rescaled parameters into the differential equations we get

$$\frac{dc}{dt} = \alpha I(1-c) + \frac{c}{\epsilon}(-K_F - K_D - K_N s - K_P(1-q)),$$

$$\frac{ds}{dt} = \frac{1}{\epsilon}\Lambda_B P_C \ c(1-s) - \lambda_r(1-q) \ s,$$

$$\frac{dq}{dt} = \frac{1}{\epsilon}K_P(1-q)\frac{P_C}{P_Q} \ c - \gamma \ q.$$

where all the parameters are of order 1. Also scaling the time $t = \epsilon\tau$, we get

$$\frac{1}{\epsilon}\frac{dc}{d\tau} = \alpha I(1-c) + \frac{c}{\epsilon}(-K_F - K_D - K_N s - K_P(1-q)),$$

$$\frac{1}{\epsilon}\frac{ds}{d\tau} = \frac{1}{\epsilon}\Lambda_B P_C \ c(1-s) - \lambda_r(1-q) \ s,$$

$$\frac{1}{\epsilon}\frac{dq}{d\tau} = \frac{1}{\epsilon}K_P(1-q)\frac{P_C}{P_Q} \ c - \gamma \ q.$$

where are the terms are of order of 1. Multiplying both sides by ϵ, the system of 3 ODEs becomes

$$\frac{dc}{d\tau} = \epsilon\alpha I(1-c) + c(-K_F - K_D - K_N s - K_P(1-q)),$$

$$\frac{ds}{d\tau} = \Lambda_B P_C \ c(1-s) - \epsilon\lambda_r(1-q) \ s,$$

$$\frac{dq}{d\tau} = K_P(1-q)\frac{P_C}{P_Q}\ c - \epsilon\gamma\ q.$$

Now we have the expansion terms

$$c = c_0 + \epsilon c_1 + \epsilon^2 c_2 + ...$$

$$s = s_0 + \epsilon s_1 + \epsilon^2 s_2 + ...$$

$$q = q_0 + \epsilon q_1 + \epsilon^2 q_2 + ...$$

where c_0, s_0 and q_0 are first terms, c_1, s_1 and q_1 are second terms and so on for the asymptotic expansion and substitute theses into the systems of 3 ODEs to get

$$\frac{dc_0}{d\tau}+\epsilon\frac{dc_1}{d\tau}+\epsilon^2\frac{dc_2}{d\tau} = \epsilon\alpha I(1-(c_0+\epsilon c_1+\epsilon^2 c_2))+(c_0+\epsilon c_1+\epsilon^2 c_2)(-K_F-K_D-K_N(s_0+\epsilon s_1+\epsilon^2 s_2)-K_P(1-(q_0+\epsilon q_1+\epsilon^2 q_2))),$$

$$\frac{ds_0}{d\tau}+\epsilon\frac{ds_1}{d\tau}+\epsilon^2\frac{ds_2}{d\tau} = \Lambda_B P_C(c_0+\epsilon c_1+\epsilon^2 c_2)(1-(s_0+\epsilon s_1+\epsilon^2 s_2))-\epsilon\lambda_r(1-(q_0+\epsilon q_1+\epsilon^2 q_2))(s_0+\epsilon s_1+\epsilon^2 s_2),$$

$$\frac{dq_0}{d\tau}+\epsilon\frac{dq_1}{d\tau}+\epsilon^2\frac{dq_2}{d\tau} = K_P(1-(q_0+\epsilon q_1+\epsilon^2 q_2))\frac{P_C}{P_Q}(c_0+\epsilon c_1+\epsilon^2 c_2) - \epsilon\gamma\ (q_0+\epsilon q_1+\epsilon^2 q_2)$$

Now, compare the coefficients by equating the powers of ϵ terms.

The ϵ^0 term gives

$$\frac{dc_0}{d\tau} = c_0(-K_F - K_D - K_N s_0 - K_P(1-q_0)), \tag{6.1}$$

$$\frac{ds_0}{d\tau} = \Lambda_B P_C\ c_0(1-s_0), \tag{6.2}$$

$$\frac{dq_0}{d\tau} = \frac{P_C}{P_Q}K_P(1-q_0)\ c_0. \tag{6.3}$$

The ϵ^1 term gives

$$\frac{dc_1}{d\tau} = \alpha I(1-c_0) + c_1(-K_F - K_D - K_N s_0 - K_P(1-q_0)) + c_0(-K_N s_1 + K_P q_1),$$

$$\frac{ds_1}{d\tau} = \Lambda_B P_C(c_1(1-s_0) - c_0 s_1) - \lambda_r(1-q_0)s_0,$$

$$\frac{dq_1}{d\tau} = \frac{P_C}{P_Q}K_P((1-q_0)c_1 - c_0 q_1) - \gamma\ q_0.$$

The ϵ^2 term gives

$$\frac{dc_2}{d\tau} = -\alpha I c_1 + c_2(-K_F - K_D - K_N s_0 - K_P(1-q_0)) - K_N(c_1 s_1 + c_0 s_2) + K_P(q_1 c_1 + q_2 c_0),$$

$$\frac{ds_2}{d\tau} = \Lambda_B P_C(c_2(1-s_0) - (c_1 s_1 + c_0 s_2)) - \lambda_r(q_1 s_0 - s_1(1-q_0),$$

$$\frac{dq_2}{d\tau} = \frac{P_C}{P_Q}K_P((1-q_0)c_2 - (q_1 c_1 + c_0 q_2)) - \gamma\ q_1.$$

With initial conditions

$$c_0(0) = c(0) = 0.0$$

$$s_0(0) = s(0) = 0.02$$

$$q_0(0) = q(0) = 0.0$$

and all other terms for c, s and q are 0 at t=0 after first terms

$$c_i(0) = 0,\ i > 0$$

$$s_i(0) = 0,\ i > 0$$

$$q_i(0) = 0, i > 0.$$

Doing the integration of equations (6.1), (6.2) and (6.3) and using the initial conditions it gives $c_0 = q_0 = 0$ and $s_0 = 0.02$ which shows that the first terms of asymptotic expansion.

Now, using the ode solver $ode23s$ with choosing $\epsilon = 10^{-9}$ in the program and substituting the values of parameters and pool values from tables (2.2) and (2.3), we generate the results for second terms (c_1, s_1, q_1) and third terms (c_2, s_2, q_2) of the asymptotic expansions.

Figure (6.1) shows that the second terms (c_1, s_1, q_1) of asymptotic expansion are non-zero terms which mean the expansion starts from second terms since they are bigger than the first terms (c_0, s_0, q_0). We also look at the third terms (c_2, s_2, q_2) of asymptotic expansion to check whether the second terms of expansion are dominate terms or not.

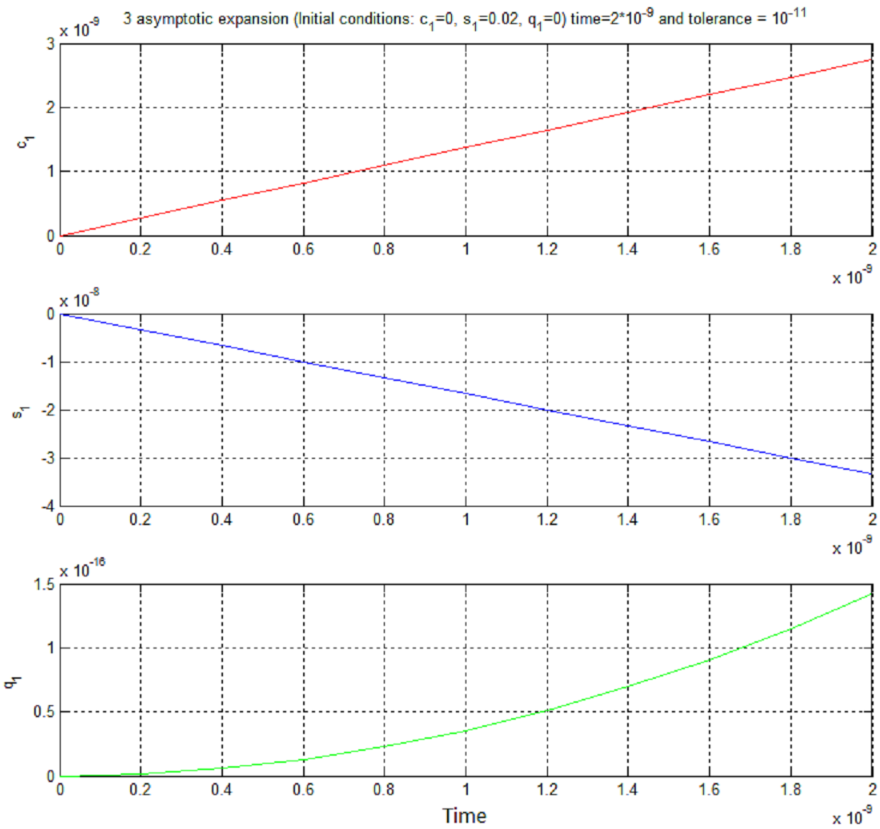

Figure 6.1: 3 Asymptotic Expansion of ODEs (c_1, s_1 and q_1) using tolerance= 10^{-11} and final time $=2 \times 10^{-9}$.

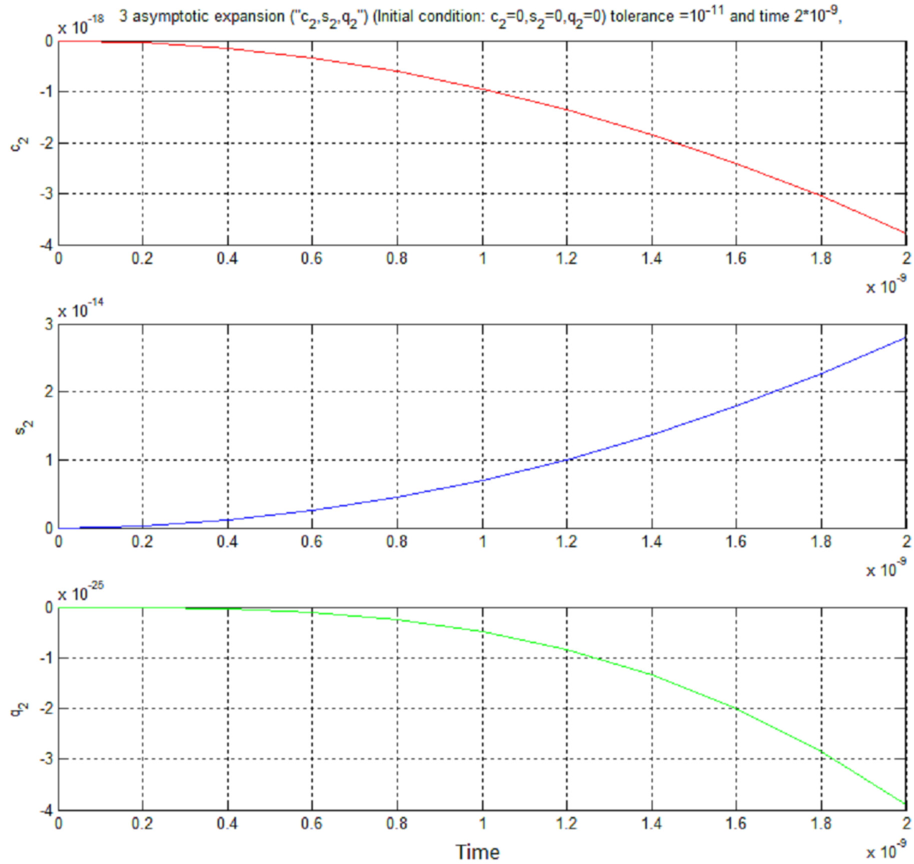

Figure 6.2: 3 Asymptotic Expansion of ODEs (c_2, s_2 and q_2) using tolerance= 10^{-11} and final time $=2 \times 10^{-9}$.

Figure (6.2) shows that the third terms (c_2, s_2 and q_2) of asymptotic expansion are non zero terms but are smaller than the second terms of the expansion. Hence, second terms (c_1, s_1 and q_1) are dominant terms in the expansion.

After the asymptotic expansion of third terms, we only keep up to second power of ϵ and ignoring after the third terms which mean expansion of c, s and q equals to

$$expansion\ of\ c = c_0 + \epsilon c_1 + \epsilon^2 c_2,$$
$$expansion\ of\ s = s_0 + \epsilon s_1 + \epsilon^2 s_2,$$
$$expansion\ of\ q = q_0 + \epsilon q_1 + \epsilon^2 q_2.$$

Now, we compared the asymptotic expansion of c, s and q with the normal ODEs of c, s and q by over plotting both of them together at different time which are presented in next page

Figure (6.3) shows this is good approximation of asymptotic for getting the 3 normal ODEs and asymptotic expansion of c, s and q same at very small time $= 2 \times 10^{-10}$. Now, we are interested to find when does theses plots start to separate when time increases?

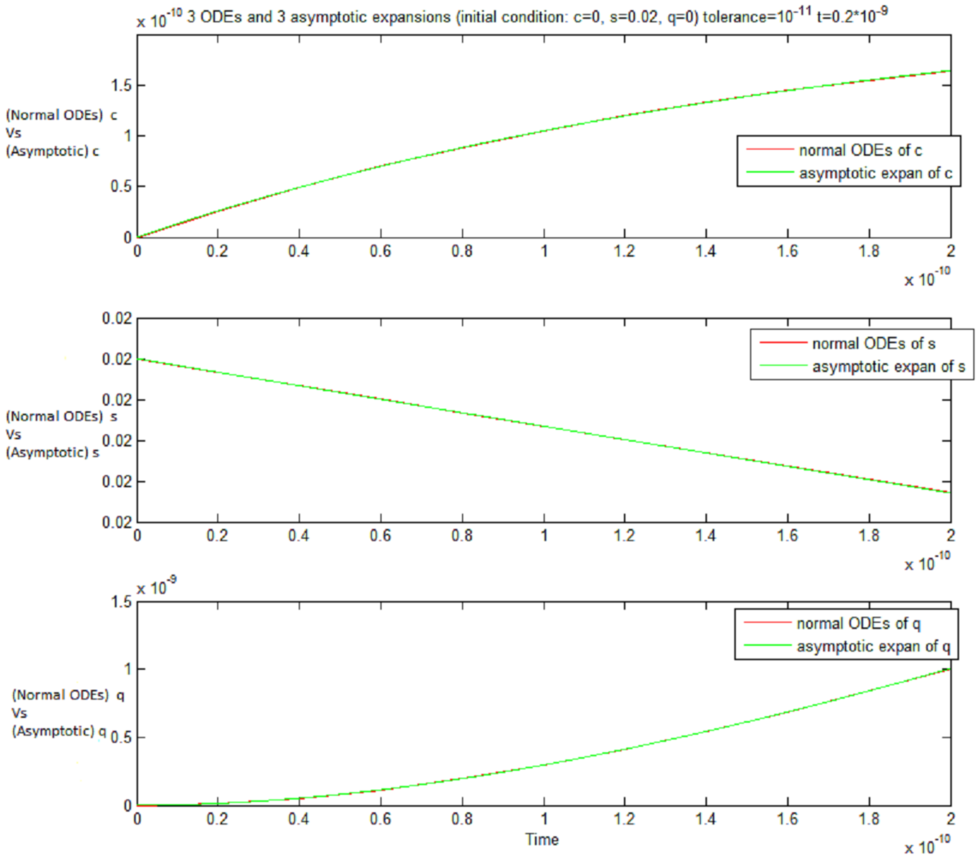

Figure 6.3: 3 Asymptotic Expansion and 3 normal ODEs of c, s and q using a final time $=2\times10^{-10}$ and tolerance$= 10^{-11}$.

Figure (6.4) shows that separation of asymptotic expansion and 3 normal ODEs when time increases at t = 2×10^{-9}.

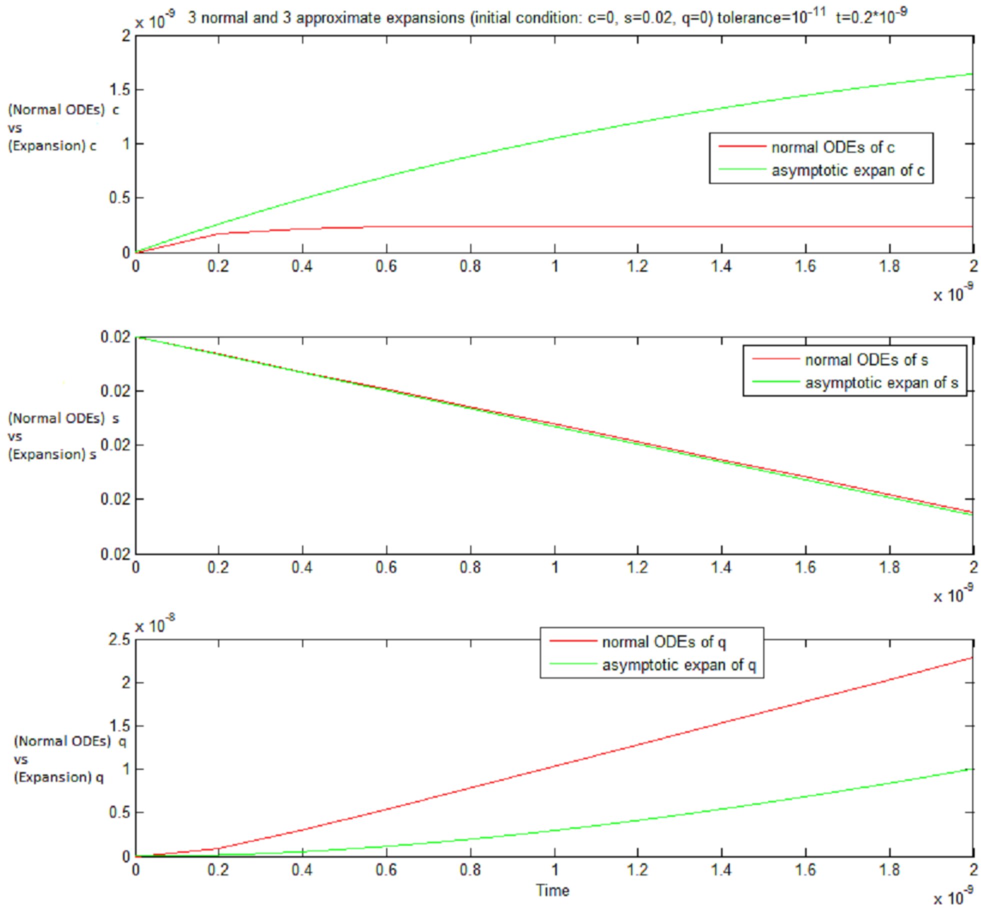

Figure 6.4: 3 Asymptotic Expansion and 3 normal ODEs of c, s and q using a final time $=2\times10^{-9}$ and tol= 10^{-11}.

In the next chapter we discuss the sensitivity of three unknown parameters of 3 nonlinear ODEs.

Chapter 7

Sensitivity to the unknown parameters for 3 ODEs

In the paper [1], they have no prior knowledge about 3 of the parameters which are γ, λ_r and λ_b which are involved in the system of nonlinear ODEs. We have therefore done a sensitivity analysis to see any significant difference in the solution of the nonlinear equations of 3 ODEs systems for c, s and q when the parameters are varied. We have changed the values of the 3 unknown parameters one at a time and plotted the results of the perturbed solutions with actual solutiions together.

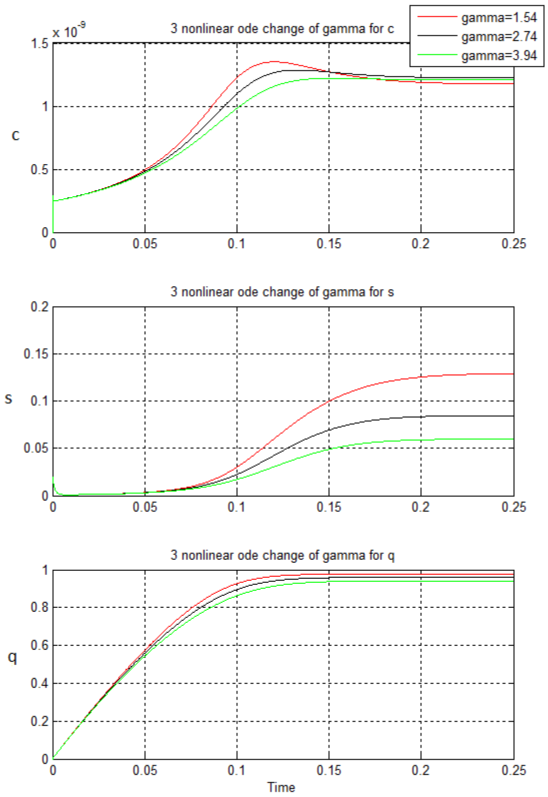

Figure 7.1: Change of γ for c, s and q in 3 ODEs.

Figure (7.1) shows the effect of perturbing initial values of γ by a small amount, as seen in the graphs, where the middle graph is the solution for the unperturbed values of γ, top and bottom are perturbed values. The changes for γ make very little significant differences for q and c compare to s.

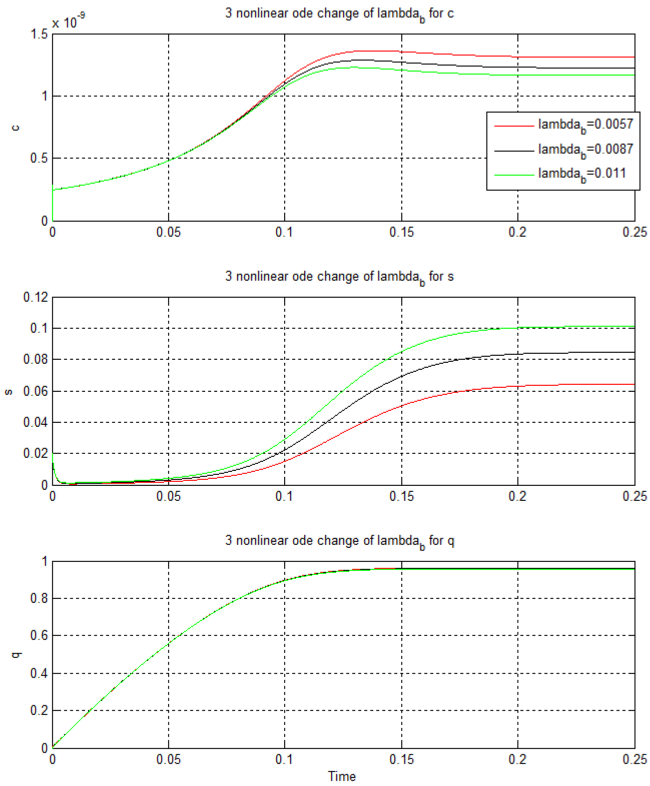

Figure 7.2: Change of λ_b for c, s and q in 3 ODEs.

Figure (7.2) shows the effect of perturbing λ_b by a small amount as seen in the graphs, where the middle graph is the solution for the unperturbed values of λ_b, top and bottom are perturbed values. The changes in λ_b give almost no significant differences for q and very little difference for c compare to s.

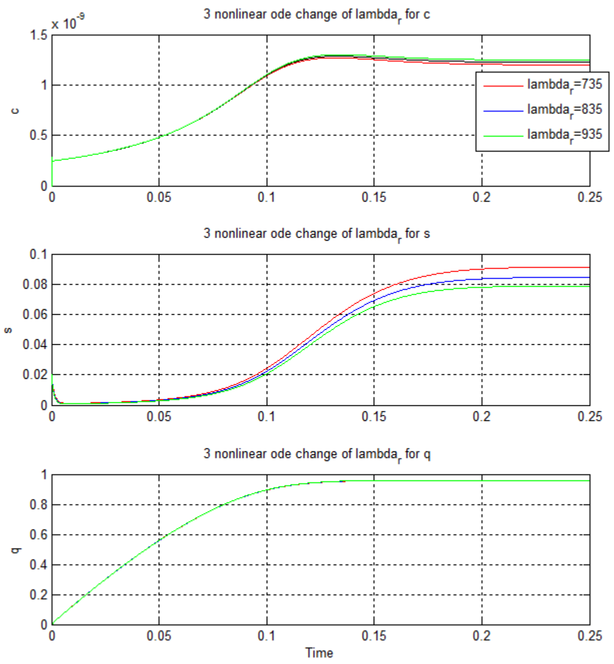

Figure 7.3: Change of λ_r for c, s and q in 3 ODEs.

Figure (7.3) shows the effect of perturbing λ_r by a small amount as seen in the graphs where the middle graph is the solution for the unperturbed values of λ_r, top and bottom are perturbed values. The changes i λ_r give no significant differences for q and less significant differences for c compared to s.

Now, from figure (7.1) with the change of γ for c, s and q, we compare between the final steady states values of perturbed and actual values and it suggest that perturbed values for γ seem to have very small effects on the actual value of γ for c and q with an error of 0.02%. It seems to have little significant differences of perturbed and actual values for s with an error of around 4%.

From figure (7.2) with the change of λ_b for c, s and q, we compare the final steady solutions of perturbed and actual values for λ_b. The perturbed values of λ_b does not have any effects on the actual value of λ_b for q and therefore no any error for q. It seems to have very little significant differences for c with an error of 0.05% and for s it has an error of 0.4%.

From figure (7.3) with the change of λ_r for c, s and q, it suggests that perturbed values for λ_r do not have any effects on the actual value of q. And for c it has a tiny effect with an error of 0.01%. There is little differences between perturbed and actual values for s with an error of around 0.03%.

Overall, there are some small significances difference for c, q and mainly for s by changing the unknown parameters of γ, λ_r and λ_b one at a time but seems to be smaller errors in total between the actual and perturbed values of the parameters. Evaluating the errors of all these parameters it suggests that, the actual values used in the paper [2] for the $\gamma = 2.74$, $\lambda_r = 835$ and $\lambda_b = 0.0087$ seems reasonale which are not sensitive when calculating the variables.

Chapter 8

Comparison of results between 3 ODEs and experiment from [1]

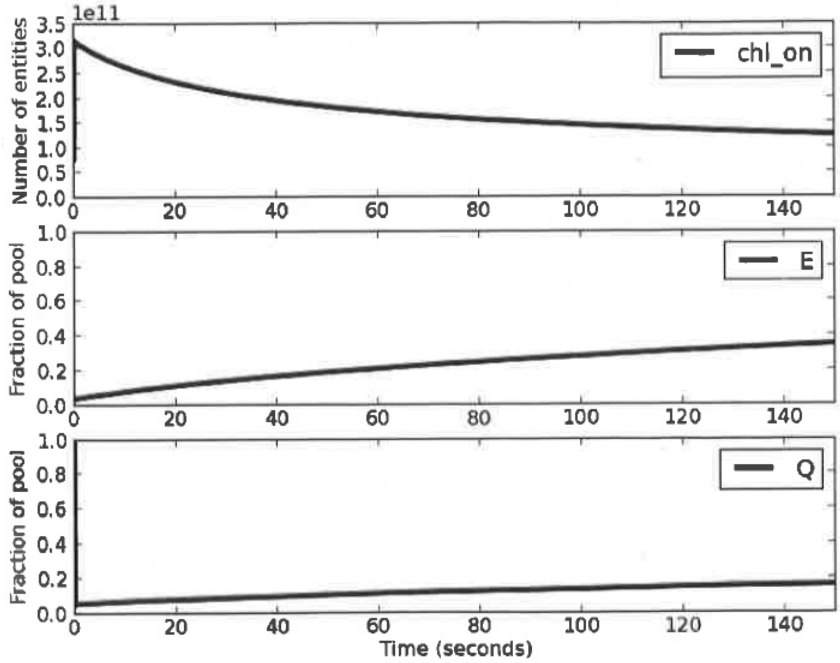

Figure 8.1: Single Model run for 3 ODEs using Euler Explicit solver with initial conditions and constant irradiance taken from [1].

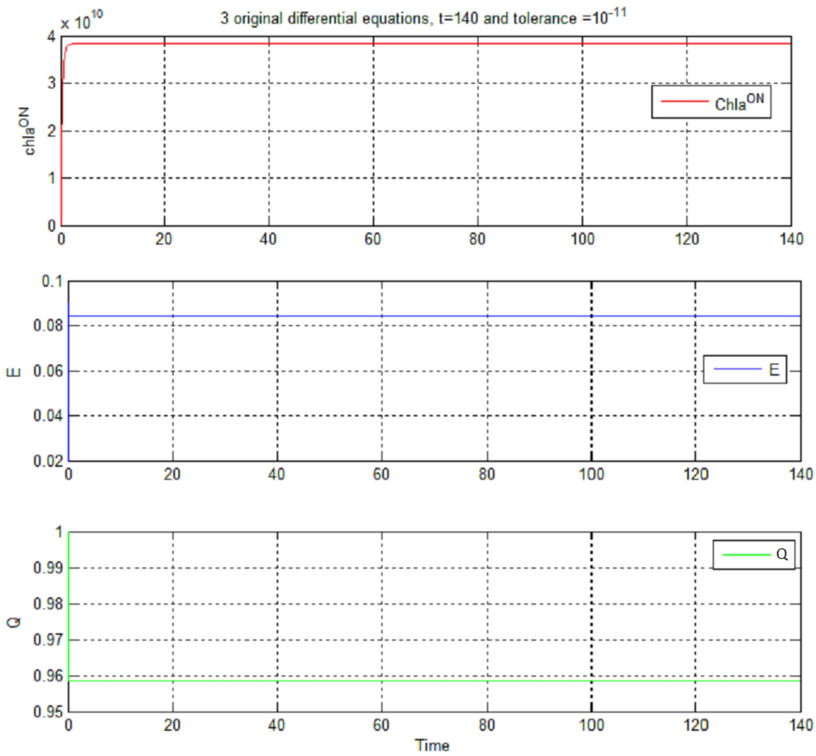

Figure 8.2: System of 3 ODEs for $Chla^{ON}$, E and Q solved by $ode23s$.

By comparing the figures (8.1) of 3 ODEs solved by $ode23s$ with the figure (8.2) of previous result of model [1], we expect Euler Scheme to give same final steady state solutions of $chla^{ON}$, E and Q as it is solved from the $ode23s$. The values of $chla^{ON}$, E and Q are still differences between these two methods although Euler Scheme has not reached the final steady state solutions.

Now, with these comparisons between figures (8.1) and (8.2), we come to the conclusion of our study where we discuss the problem of solving systems of 3 nonlinear ODEs by using Explicit Euler scheme and relate it to our solution.

Chapter 9

Conclusion and future work

In the model [1], the system of 3 nonlinear ODEs was solved by the Explicit Euler method. Here, we address the problem of solving the system numerically by a stiff solver. First we showed that the system has a unique stable steady state. Then we determined the stiffness and used a stiff solver $ode23s$ from MATLAB. The system of 3 ODEs can be reduced to system of 2 ODEs. We also clarified about the unknown parameters that have been used in [1] to solve the system of 3 ODEs by doing sensitivity perturbations and comparing the significance differences between actual and perturbed values of unknown parameters. We now summarize the results we have found and discuss some ideas for further work.

9.1 Summary of the results

The results of this research are particularly interesting in the application to this system of ordinary differential equations. First we non-dimensionalised the system and worked with the non-dimensionalised variables c, s and q.

In the third chapter, from the Descartes rule of signs we showed that there is only one positive steady-states for c, s and q which lies between 0 and 1. We used the Newton-Raphson method to find the unique steady-state of 3 ODEs system and found the stability of the steady-state which proved steady state is stable. This shows that the steady state we found using Newton-Raphson method is ‘correct’.

In chapter 4, by finding the condition number of the Jacobian for the 3 ODEs we found out that the system of 3 ODEs is an extremely stiff system. So, we used the stiff solver $ode23s$ from MATLAB to solve the system of 3 ODEs and manipulated the tolerance to get good results for the components c, s and q. Since c was changing very quickly at first, we looked at the behaviour of c using the final time $=10^{-8}$ and choosing tolerance $=10^{-11}$ to get a smooth graph of c which showed how c was behaving initially. The final steady solutions of 3 ODEs for c, s and q are almost exactly the same as the steady states of c, s and q which were found by using the Newton-Raphson method.

In chapter 5, we assumed that $\frac{dc}{dt}$ was zero after a small time and reduced the system of 3 ODEs to 2 ODEs and then applied the same methods to find the steady-state and stability of the system of 2 ODEs and the steady state results obtained for 2 ODEs were the same as the system of 3 ODEs. However, the system of 2 ODEs is less stiff compared to that of the 3 ODEs. Then, we used the program $ode23s$ to solve the system of 2 ODEs and got the same results for s and q. In the system of 2 ODEs the behaviour of c was progressing less quickly as than in 3 ODEs and the starting point of initial condition was different. From these results, we can be confident enough to use the 2 ODEs rather than 3 ODEs to get a good solution of the system after a short time. The system of 2 ODEs does not require us to deal with the rapidly changing behaviour of c at the initial time which was causing the system of 3 ODEs to be extra stiff.

Descartes rule of signs shows that the solutions were unique and both methods Newton Raphson method and $ode23s$ stiff solver gave the same steady-state solution. With these results we have found that both methods are successful methods to get correct numerical solutions for solving the nonlinear systems of ODEs after a short time.

We have also done an asymptotic expansion of the 3 ODEs system in chapter 6 to see the detailed behaviour of the system close to the initial state. We approached the asymptotic expansion by spotting the dominant terms and scaling the larger parameters to get a good expansion. Then using the ode solver $ode23s$ by choosing a fine tolerance 10^{-11}, we compared the results of the asymptotic expansions with system of 3 ODEs. We compared them and they compared well because we managed to find asymptotic expansion of 3 ODEs and normal 3 ODEs equal at the very small time $= 10^{-10}$ and as time increase around $t=10^{-9}$ we got their separation point which indicates good approximation of asymptotic expansion. This also shows that asymptotic expansion of 3 ODEs was successfully calculated at the initial state of the system.

In chapter 7, we did sensitivity to unknown parameters of ODEs and compared the perturbed values and actual values of parameters, it does not have any big significances difference between perturbed values and actual values of γ, λ_b and λ_r for c, s and q. Hence, there is little effect on the system of 3 ODEs and we assume that the values they have used for the γ, λ_b and λ_r in the model [1] are adequate.

In chapter 8, we compared the results of the system of 3 ODEs with the results of model [1]. From these comparison, the model [1] and system 3 ODEs solved by $ode23s$, gave different solutions and hence we conclude that there are definitely errors in the results of the model [1] which was solved by using the Explicit Euler scheme, because Euler method gives less accurate solutions, particularly for stiff systems.

The goals of the dissertation were

- an investigation of steady-state, stability and stiffness of systems of 3 and 2 ODEs,
- to generalize known results of 2 and 3 ODEs and compare between them,
- to study the problem of the asymptotic behaviour of solutions initially,
- to find the sensitivity to unknown parameters of 3 ODEs
- to compare with experiment of the model [1].

In this dissertation, we have looked mainly at a model of photosystem II and tried with an analytical way like Descartes rule of signs to find the steady state of the system of non-linear ODEs. We have demonstrated that the MATLAB ode solver $ode23s$ is a very powerful technique to solve non-linear system of ODEs numerically and particularly for the stiff problems. Therefore, $ode23s$ were required for these stiff problems to get efficient solution while Explicit Euler method will not able to provide accurate solutions. Though the nonlinear differential equations can be solved initially by using various numerical schemes, asymptotic expansion techniques provide an awareness of the solution before one computes the numerical solution. We also looked at sensitivity to unknown parameters of 3 ODEs to eliminate an error for the unknown parameters.

Overall, the dissertation has successfully presented numerical results for this system of nonlinear ODEs. The steady-state results calculated from Newton-Raphson method and results from the dynamic approached calculated from $ode23s$ gave the same solutions which is satisfactory point for the dissertation. The stability condition suggests that the system of ODEs is stable which is also satisfactory for the dissertation.

Comparing the results of model [1] run by a dynamic approach using Explicit Euler scheme and our dynamic approach run by stiff solver $odes23s$, all the explicit schemes suffer from a limitation of the time step for the reasons of instability. Since the previous work was done under light changing conditions occurring at a time scale of few seconds [1], it is very important to understand the concepts of short time behavior of system at the initial state, since it is a stiff systems of ODEs. In addition, from the background of study [2] they have compared the analysis of dynamic approach against steady state approach and have chosen dynamic approach as better. From our research, using the dynamic approach we can see the results of initial behaviour of the system before we get the solutions after a short time.

9.2 Further work

The ideas for extending the work in this project now can be done by using 2 ODEs model to solve the systems. In chapter 6 asymptotic analysis of 3 ODEs was done. Similarly, an asymptotic analysis of the system of 2 ODEs would be interesting to see the behaviour of s and q at the initial states, which could lead to an improvement in the results. Due to time limitation we were unable to look at matched asymptotic expansions of 3 ODES.

Bibliography

[1] J.Atherton. A simple model of light use in Photosystem II. Private Communication

[2] A.Porcar-Castell,J.Black,E. Juurola, and P.Hari. Dynamics of the energy flow through photosystem II under changing light conditions:a model approach. Functioanl Plant Biology 33(3):pp229-239,2006.

[3] Lawlor, D.W., Photosynthesis : Molecular, Physiological and Environmental Processes 2nd edition, Longman Group, London, 1993, Chapter 2

[4] George, C.P. and Govindjee, Chlorophyll a Fluorescence : A Signature of Photosynthesis, Springer, 2004, Chapter 1

[5] `http://www.sciencedirect.com/science/article/pii/S1360138510002116/`

[6] Griffiths, D.F. and Higham, D.J., Numerical Methods for Ordinary Differential Equations, Springer, London, 2010, Chapters 7, 8 and 10.

[7] Dahlquist, G. and Bjorck, A., Numerical Methods, Dover, New york, 2003, Chapter 6

[8] `http://www.mathplanet.com/education/algebra-2/polynomial-functions/descartes%C2%B4rule-of-sign`

[9] `http://pages.jh.edu/~motn/relevantnotes/usingmatlab_ode.pdf`

[10] L.F. Shampine, Numerical Solution of Ordinary Differential Equations,Chapman Hall, New York, 1994

[11] Higham, D.J. and Higham, N.J., MATLAB GUIDE, siam, Philadelphia, 2000, Chapter 12

[12] Biggs, N.R., University of Reading, MA3AM1/MAMA13 Asymptotic Methods I Lecture notes, 2009

[13] Tayler, A.B., Mathematical Models in Applied Mechanics, Oxford, 1984, Chapter 6

[14] `http://www.mathworks.co.uk/help/simulink/ug/choosing-a-solver.html`